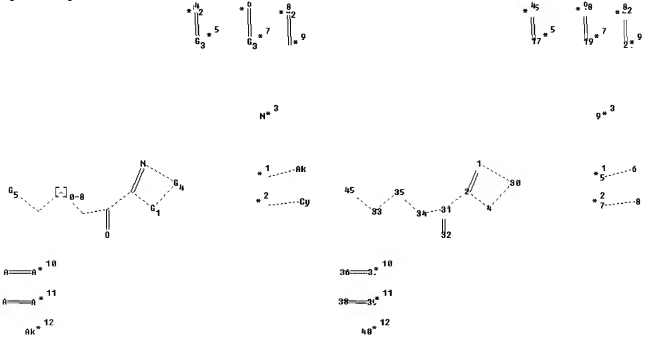
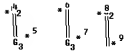
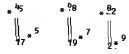
```
=> file registry
FILE 'REGISTRY' ENTERED AT 10:04:47 ON 08 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:    7 OCT 2008  HIGHEST RN 1058345-57-5
DICTIONARY FILE UPDATES:   7 OCT 2008  HIGHEST RN 1058345-57-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html
Uploading L10.str
```

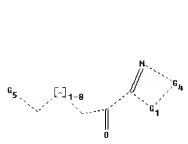


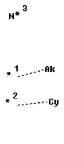
```
chain nodes :
6  8  31  32  33  34  35  40  45
ring nodes :
1  2  4  5  7  9  15  17  18  19  21  22  30
ring/chain nodes :
36  37  38  39
chain bonds :
2-31  5-6  7-8  31-32  31-34  33-35  33-45  34-35
ring/chain bonds :
```

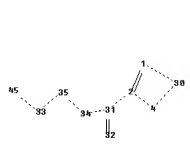
```
36-37  38-39
ring bonds :
1-2  1-30  2-4  4-30  15-17  18-19  21-22
exact/norm bonds :
1-2  1-30  2-4  2-31  4-30  5-6  7-8  15-17  18-19  21-22  31-32  31-34  33-35  33-
45
34-35  36-37
exact bonds :
38-39


G1:O,S

G2:[*1],[*2],[*3]

G3:[*1],[*2]

G4:[*4-*5],[*6-*7],[*8-*9]

G5:[*10],[*11],[*12]

Connectivity :
9:2 E exact RC ring/chain  18:2 E exact RC ring/chain  21:2 E exact RC ring/chain

Match level :
1:Atom  2:Atom  4:Atom  5:Atom  6:CLASS  7:Atom  8:Atom  9:Atom  15:Atom  17:Atom
18:Atom  19:CLASS  21:Atom  22:CLASS  30:Atom  31:CLASS  32:CLASS  33:CLASS
34:CLASS  35:CLASS
36:CLASS  37:CLASS  38:CLASS  39:CLASS  40:CLASS  45:CLASS
Generic attributes :
8:
Saturation              : Unsaturated



Uploading L25.str
```

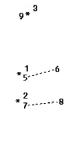












```
chain nodes :
6  8  31  32  33  34  35  40  45
ring nodes :
1  2  4  5  7  9  15  17  18  19  21  22  30
ring/chain nodes :
36  37  38  39
chain bonds :
2-31  5-6  7-8  31-32  31-34  33-35  33-45  34-35
ring/chain bonds :
36-37  38-39
ring bonds :
1-2  1-30  2-4  4-30  15-17  18-19  21-22
exact/norm bonds :
1-2  1-30  2-4  2-31  4-30  5-6  7-8  15-17  18-19  21-22  31-32  31-34  33-35  33-
45
34-35  36-37
exact bonds :
38-39


G1:O,S

G2:[*1],[*2],[*3]

G3:[*1],[*2]

G4:[*4-*5],[*6-*7],[*8-*9]

G5:[*10],[*11],[*12]

Connectivity :
6:1 E exact RC ring/chain  9:2 E exact RC ring/chain  18:2 E exact RC ring/chain
21:2 E exact RC ring/chain  40:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  4:Atom  5:Atom  6:CLASS  7:Atom  8:Atom  9:Atom  15:Atom  17:Atom
18:Atom  19:CLASS  21:Atom  22:CLASS  30:Atom  31:CLASS  32:CLASS  33:CLASS
34:CLASS  35:CLASS
36:CLASS  37:CLASS  38:CLASS  39:CLASS  40:CLASS  45:CLASS
Generic attributes :
8:
Saturation             : Unsaturated




=> file zcaplus
FILE 'ZCAPLUS' ENTERED AT 10:04:50 ON 08 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
```

databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS is strictly prohibited.

FILE COVERS 1907 - 8 Oct 2008 VOL 149 ISS 15
FILE LAST UPDATED: 7 Oct 2008 (20081007/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L31
L10 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

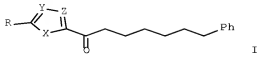
Structure attributes must be viewed using STN Express query preparation.
L12 1689 SEA FILE=REGISTRY SSS FUL L10
L25 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L27 373 SEA FILE=REGISTRY SUB=L12 SSS FUL L25
L29 106 SEA FILE=REGISTRY ABB=ON PLU=ON L27 AND N2COC/ES
L30 267 SEA FILE=REGISTRY ABB=ON PLU=ON L27 NOT L29
L31 35 SEA FILE=ZCAPLUS ABB=ON PLU=ON L30

=> d ibib abs hitstr L31 1-35

L31 ANSWER 1 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:859432 ZCAPLUS Full-text
DOCUMENT NUMBER: 149:224187
TITLE: Optimization of the Central Heterocycle of α-Ketoheterocycle Inhibitors of Fatty Acid Amide Hydrolase
AUTHOR(S): Garfunkle, Joie; Ezzili, Cyrine; Rayl, Thomas J.; Hochstatter, Dustin G.; Hwang, Inkyu; Boger, Dale L.
CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of Medicinal Chemistry (2008), 51(15), 4392-4403
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

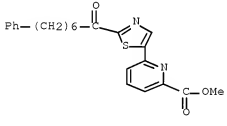


I

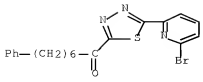
AB The synthesis and evaluation of a refined series of α- ketoheterocycles based on the oxazole I (R = 2-pyridyl, X = O, Y = CH, Z = N) (II) (OL-135) incorporating systematic changes in the central heterocycle bearing a key set of added substituents are described. The nature of the central heterocycle, even within the systematic and minor perturbations explored herein, significantly influenced the inhibitor activity: 1,3,4-oxadiazoles and 1,2,4-oxadiazoles I (R = H, 2-pyridyl, 2-furanyl, etc., X = Y = N, Z = O) (III) > tetrazoles, the isomeric 1,2,4-oxadiazoles I (X = Z = N, Y = O) (IV), 1,3,4-thiadiazoles > oxazoles including II > 1,2-diazines > thiazoles > 1,3,4-triazoles. Most evident in these trends is the observation that introduction of an addnl. heteroatom at position 4 (oxazole numbering, N > O > CH) substantially increases activity that may be attributed to a reduced destabilizing steric interaction at the FAAH active site. Added heterocycle substituents displaying well-defined trends may be utilized to enhance the inhibitor potency and, more significantly, to enhance the inhibitor selectivity. These trends, exemplified herein, emerge from both enhancements in the FAAH activity and simultaneous disruption of binding affinity for competitive off-target enzymes.

IT 1042152-50-0P 1042152-62-4P 1042152-64-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation and SAR of α-ketoheterocycles as fatty acid amide hydrolase inhibitors)

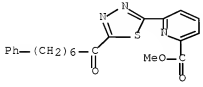
RN 1042152-50-0 ZCAPLUS
CN INDEX NAME NOT YET ASSIGNED



RN 1042152-62-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(6-bromo-2-pyridinyl)-1,3,4-thiadiazol-2-yl]-7-phenyl- (CA INDEX NAME)

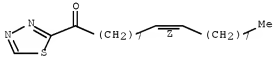


RN 1042152-64-6 ZCAPLUS
CN INDEX NAME NOT YET ASSIGNED

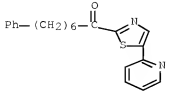


IT 681135-38-6P 1042152-40-8P 1042152-45-3P
1042152-48-6P 1042152-51-1P 1042152-56-6P
1042152-57-7P 1042152-59-9P 1042152-60-2P
1042152-61-3P 1042152-65-7P 1042152-69-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and SAR of α-ketoheterocycles as fatty acid amide hydrolase inhibitors)
RN 681135-38-6 ZCAPLUS
CN 9-Octadecen-1-one, 1-(1,3,4-thiadiazol-2-yl)-, (9Z)- (CA INDEX NAME)

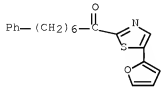
Double bond geometry as shown.



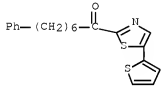
RN 1042152-40-8 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-thiazolyl]- (CA INDEX NAME)



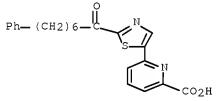
RN 1042152-45-3 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-furanyl)-2-thiazolyl]-7-phenyl- (CA INDEX NAME)



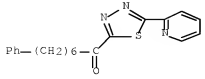
RN 1042152-48-6 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-thienyl)-2-thiazolyl]- (CA INDEX NAME)



RN 1042152-51-1 ZCAPLUS
CN INDEX NAME NOT YET ASSIGNED

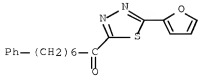


RN 1042152-56-6 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-1,3,4-thiadiazol-2-yl]- (CA INDEX NAME)



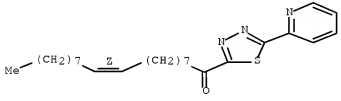
RN 1042152-57-7 ZCAPLUS

CN 1-Heptanone, 1-[5-(2-furanyl)-1,3,4-thiadiazol-2-yl]-7-phenyl- (CA INDEX NAME)



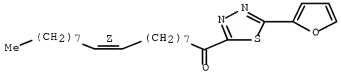
RN 1042152-59-9 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-pyridinyl)-1,3,4-thiadiazol-2-yl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

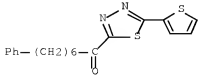


RN 1042152-60-2 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-furanyl)-1,3,4-thiadiazol-2-yl]-, (9Z)- (CA INDEX NAME)

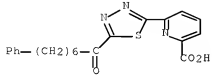
Double bond geometry as shown.



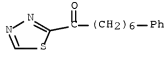
RN 1042152-61-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-thienyl)-1,3,4-thiadiazol-2-yl]- (CA INDEX NAME)



RN 1042152-65-7 ZCAPLUS
CN INDEX NAME NOT YET ASSIGNED



RN 1042152-69-1 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-(1,3,4-thiadiazol-2-yl)- (CA INDEX NAME)



REFERENCE COUNT: 98 THERE ARE 98 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

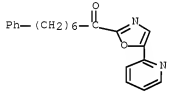
L31 ANSWER 2 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:836914 ZCAPLUS Full-text
DOCUMENT NUMBER: 149:324443
TITLE: Fatty acid amide hydrolase inhibition enhances the anti-allodynic actions of endocannabinoids in a model of acute pain adapted for the mouse
AUTHOR(S): Palmer, J. A.; Higuera, E. S.; Chang, L.; Chaplan, S. R.
CORPORATE SOURCE: Pain and Related Disorders, Johnson & Johnson Pharmaceutical Research and Development, L.L.C., San Diego, CA, 92121, USA
SOURCE: Neuroscience (Oxford, United Kingdom) (2008), 154(4), 1554-1561
CODEN: NRSCDN; ISSN: 0306-4522
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cannabinoid ligands have been shown to be anti-nociceptive in animal models of acute and chronic pain by acting at the two known cannabinoid receptors, cannabinoid-1 receptor (CB-1) and cannabinoid-2 receptor (CB-2). A major concern with the use of cannabinoids for pain relief is that they activate receptors at sites other than those involved in the transmission of nociceptive stimuli. An alternative approach is to target the naturally occurring endocannabinoids, such as anandamide (AEA), 2-arachidonylglycerol (2-AG) and N-arachidonylglycine (N-AG). However in vivo results obtained with these compds. appear to be weak, most probably due to their rapid degradation and subsequent short half-life. The predominant enzyme responsible for the hydrolysis of anandamide (and some other endocannabinoids) in the brain is fatty acid amide hydrolase (FAAH). Recently, the α-ketoheterocycle OL135 has been synthesized and shown to be a highly potent and selective inhibitor of

FAAH with efficacy in pain models in vivo. In the present study, we have adapted the mild thermal injury (MTI) model of acute pain for the mouse and pharmacol. characterized this model by showing significant reversal of the tactile allodynia by morphine (3, 5 and 10 mg kg-1 s.c.), gabapentin (100 and 300 mg kg-1 i.p.), ibuprofen (100 mg kg-1 i.p.) and OL135 (10, 30 and 100 mg kg-1 i.p.). Furthermore we have demonstrated, using this model, that a subtherapeutic dose of OL135 can enable the endocannabinoids AEA and 2-AG, but not N-AG to be active at doses where they are otherwise nonanalgesic (20 mg kg-1 i.p.). The implications of this model in the study of pain in mice, and the therapeutic potential of FAAH inhibition to provide analgesia without the undesirable side effects of direct agonism of cannabinoid receptors are discussed.

IT 681135-77-3, OL135
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fatty acid amide hydrolase inhibition enhances the anti-allodynic actions of endocannabinoids in a model of acute pain adapted for the mouse)

RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



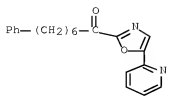
L31 ANSWER 3 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:338585 ZCAPLUS Full-text
DOCUMENT NUMBER: 148:528850
TITLE: Novel ketooxazole based inhibitors of fatty acid amide hydrolase (FAAH)
AUTHOR(S): Timmons, Amy; Seierstad, Mark; Apodaca, Rich; Epperson, Matt; Pippel, Dan; Brown, Sean; Chang, Leon; Scott, Brian; Webb, Michael; Chaplan, Sandra R.; Breitenbucher, J. Guy
CORPORATE SOURCE: Johnson & Johnson Pharmaceutical Research and Development, L.L.C., San Diego, CA, 92121, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(6), 2109-2113
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Efforts to improve the properties of the well studied ketooxazole FAAH inhibitor OL-135 resulted in the discovery of a novel propylpiperidine series of FAAH inhibitors that has a modular design and superior properties to OL-135. The efficacy of one of these compds. was demonstrated in a rat spinal nerve ligation model of neuropathic pain in rats.

IT 681135-77-3, OL-135
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel ketooxazole-based inhibitors of fatty acid amide hydrolase)

RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



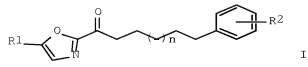
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 4 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:318656 ZCAPLUS Full-text
DOCUMENT NUMBER: 148:331666
TITLE: Preparation of oxazole derivatives as fatty acid amide hydrolase inhibitors
INVENTOR(S): Boger, Dale L.
PATENT ASSIGNEE(S): The Scripps Research Institute, USA
SOURCE: PCT Int. Appl., 58pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

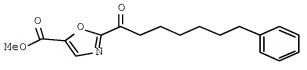
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008030532	A2	20080313	WO 2007-US19471	20070907
WO 2008030532	A3	20080912		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2006-843277P P 20060908
OTHER SOURCE(S): MARPAT 148:331666
GI



I



II

AB The title compds. with general formula I [wherein n = 0-3; R1 = CF3, CN, CHO, (un)substituted C(=O)alkyl, etc.; R2 = H, alkyl, cycloalkyl, CF3, etc.] or pharmaceutically acceptable salts, prodrugs, or pharmaceutically active metabolites thereof were prepared, which are useful as fatty acid amide hydrolase (FAAH) inhibitors. Thus, I may be administered for the treatment of anxiety, pain, inflammation, sleep disorders, eating disorders, or movement disorders (such as multiple sclerosis), etc. For example, 2-[1-(tert-butyldimethylsilyloxy)-7-phenylheptyl]oxazole was first treated with tert-Bu lithium in anhydrous THF at -78 °C under argon and then reacted with carbon dioxide to afford 2-[1-(tert- butyldimethylsilyloxy)-7-phenylheptyl]oxazole-5-carboxylic acid. The intermediate obtained above was reacted with methanol and then de-protected to give II as a final product.

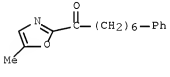
IT 914493-10-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of oxazole derivs. as fatty acid amide hydrolase inhibitors)

RN 914483-10-6 ZCAPLUS

CN 1-Heptanone, 1-(5-methyl-2-oxazolyl)-7-phenyl- (CA INDEX NAME)



L31 ANSWER 5 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:141098 ZCAPLUS Full-text

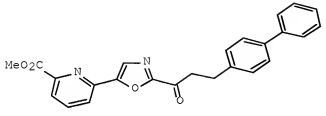
DOCUMENT NUMBER: 148:379521

TITLE: Optimization of α-Ketooxazole Inhibitors of Fatty Acid Amide Hydrolase

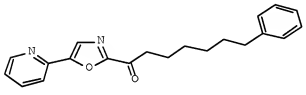
AUTHOR(S): Kimball, F. Scott; Romero, F. Anthony; Ezzili, Cyrine; Garfunkle, Joie; Rayl, Thomas J.; Hochstatter, Dustin G.; Hwang, Inkyu; Boger, Dale L.

CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La

Jolla, CA, 92037, USA
SOURCE: Journal of Medicinal Chemistry (2008), 51(4), 937-947
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:379521
GI

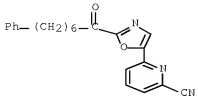


I

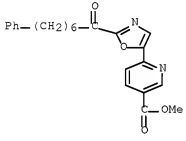


II

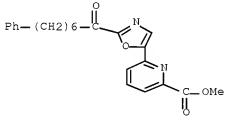
AB A series of α-ketooxazoles, e.g., I, containing conformational constraints in the flexible C2 acyl side chain of II (OL-135) and representative oxazole C5 substituents were prepared and examined as inhibitors of fatty acid amide hydrolase (FAAH). Exceptionally potent and selective FAAH inhibitors emerged from the series (e.g., 6, Ki = 200 and 260 pM for rat and rhFAAH). With simple and small C5 oxazole substituents, each series bearing a biphenylethyl, phenoxyphenethyl, or (phenoxymethyl)phenethyl C2 side chain was found to follow a well-defined linear relationship between -log Ki and Hammett σp of a magnitude (ρ = 2.7-3.0) that indicates that the substituent electronic effect dominates, confirming its fundamental importance to the series and further establishing its predictive value. Just as significantly, the nature of the C5 oxazole substituent substantially impacts the selectivity of the inhibitors whereas the effect of the C2 acyl chain was more subtle but still significant even in the small series examined Combination of these independent features, which display generalized trends across a range of inhibitor series, simultaneously improves FAAH potency and selectivity and can provide exquisitely selective and potent FAAH inhibitors.
IT 1012329-34-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation, fatty acid amide hydrolase inhibitory activity, and SAR of ketooxazoles)
RN 1012329-34-8 ZCAPLUS
CN 2-Pyridinecarbonitrile, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



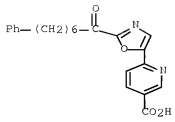
IT 935264-42-9P 935264-43-0P 935264-46-3P
935264-47-4P 1012329-35-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, fatty acid amide hydrolase inhibitory activity, and SAR of ketooxazoles)
RN 935264-42-9 ZCAPLUS
CN 3-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



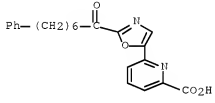
RN 935264-43-0 ZCAPLUS
CN 2-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



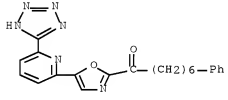
RN 935264-46-3 ZCAPLUS
CN 3-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



RN 935264-47-4 ZCAPLUS
CN 2-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



RN 1012329-35-9 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-[6-(2H-tetrazol-5-yl)-2-pyridinyl]-2-oxazolyl]- (CA INDEX NAME)



REFERENCE COUNT: 87 THERE ARE 87 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

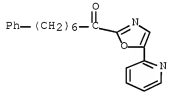
L31 ANSWER 6 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1181860 ZCAPLUS Full-text
DOCUMENT NUMBER: 148:23752
TITLE: Novel Mechanistic Class of Fatty Acid Amide Hydrolase Inhibitors with Remarkable Selectivity
AUTHOR(S): Ahn, Kyunghye; Johnson, Douglas S.; Fitzgerald, Laura R.; Liimatta, Marya; Arendse, Andrea; Stevenson, Tracy; Lund, Eric. T.; Nugent, Richard A.; Nomanbhoy, Tyzoon K.; Alexander, Jessica P.; Cravatt, Benjamin F.
CORPORATE SOURCE: Pfizer Global Research and Development, Ann Arbor, MI, 48105, USA
SOURCE: Biochemistry (2007), 46(45), 13019-13030

CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fatty acid amide hydrolase (FAAH) is an integral membrane enzyme that degrades the fatty acid amide family of signaling lipids, including the endocannabinoid anandamide. Genetic or pharmacol. inactivation of FAAH leads to analgesic, anti-inflammatory, anxiolytic, and antidepressant phenotypes in rodents without showing the undesirable side effects observed with direct cannabinoid receptor agonists, indicating that FAAH may represent an attractive therapeutic target for treatment of pain, inflammation, and other central nervous system disorders. However, the FAAH inhibitors reported to date lack drug-like pharmacokinetic properties and/or selectivity. Herein the authors describe piperidine/piperazine ureas represented by N-phenyl-4-(quinolin-3-ylmethyl)piperidine-1- carboxamide (PF-750) and N-phenyl-4-(quinolin-2-ylmethyl)piperazine-1- carboxamide (PF-622) as a novel mechanistic class of FAAH inhibitors. PF-750 and PF-622 show higher in vitro potencies than previously established classes of FAAH inhibitors. Rather unexpectedly based on the high chemical stability of the urea functional group, PF-750 and PF-622 were found to inhibit FAAH in a time-dependent manner by covalently modifying the enzyme's active site serine nucleophile. Activity-based proteomic profiling revealed that PF-750 and PF-622 were completely selective for FAAH relative to other mammalian serine hydrolases. The authors hypothesize that this remarkable specificity derives, at least in part, from FAAH's special ability to function as a C(O)-N bond hydrolase, which distinguishes it from the vast majority of metabolic serine hydrolases in mammals that are restricted to hydrolyzing esters and/or thioesters. The piperidine/piperazine urea may thus represent a privileged chemical scaffold for the synthesis of FAAH inhibitors that display an unprecedented combination of potency and selectivity for use as potential analgesic and anxiolytic/antidepressant agents.

IT 681135-77-3, OL-135
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel mechanistic class of fatty acid amide hydrolase inhibitors with remarkable selectivity)

RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



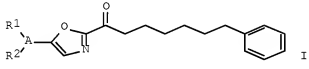
REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

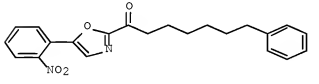
L31 ANSWER 7 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:970784 ZCAPLUS Full-text
DOCUMENT NUMBER: 147:322968
TITLE: Preparation of keto-oxazole compounds as modulators of fatty acid amide hydrolase
INVENTOR(S): Boger, Dale L.

PATENT ASSIGNEE(S): The Scripps Research Institute, USA
SOURCE: PCT Int. Appl., 85pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007098142	A2	20070830	WO 2007-US4341	20070220
WO 2007098142	A3	20080904		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			
AU 2007217813	A1	20070830	AU 2007-217813	20070220
US 20070203156	A1	20070830	US 2007-708788	20070220
PRIORITY APPLN. INFO.:			US 2006-774322P P	20060217
			WO 2007-US4341 W	20070220

OTHER SOURCE(S): MARPAT 147:322968
GI


I

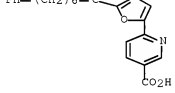

II

AB Title compds. I [R1 = alkyl, cycloalkyl, CF3, CN, OH, halo, etc.; R2 = H, alkyl, cycloalkyl, CF3, CN, NO2, etc.; ring A = 5- to 6-membered aryl or heteroaryl], and their pharmaceutically acceptable salts, prodrugs or active metabolites are prepared and disclosed as modulators of fatty acid amide hydrolase (FAAH). Thus, e.g., Stille coupling reaction of 2-[1-[(tert-butyldimethylsilyl)oxy]-7-phenylheptyl]-5- (tributylstannyl)oxazole with 1-iodo-2-nitrobenzene followed by deprotection and oxidation provided II. Select invention compds. were evaluated for their inhibitory activity on FAAH, II exhibited IC50 value of 340 nM in human FAAH assay.. I may be useful for

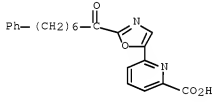
the treatment of disease states, disorders, and conditions mediated by FAAH activity, such as anxiety, pain, inflammation, sleep disorders, eating disorders, or movement disorders.

IT 935264-45-3P, 6-[2-(7-Phenylheptanoyl)oxazol-5-yl]nicotinic acid 935264-47-4P, 6-[2-(7-Phenylheptanoyl)oxazol-5-yl]picolinic acid
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of keto-oxazole compds. as modulators of fatty acid amide hydrolase)

RN 935264-46-3 ZCAPLUS
CN 3-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



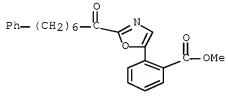
RN 935264-47-4 ZCAPLUS
CN 2-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



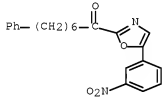
IT 935263-94-6P, Methyl 2-[2-(7-phenylheptanoyl)oxazol-5-yl]benzoate 935264-01-0P, 1-[5-(3-Nitrophenyl)oxazol-2-yl]-7-phenylheptan-1-one 935264-05-4P, Methyl 3-[2-(7-phenylheptanoyl)oxazol-5-yl]benzoate 935264-19-0P, 1-[5-(4-Nitrophenyl)oxazol-2-yl]-7-phenylheptan-1-one 935264-21-4P, Methyl 4-[2-(7-phenylheptanoyl)oxazol-5-yl]benzoate 935264-37-2P, 1-[5-(4-Nitropyridin-2-yl)oxazol-2-yl]-7-phenylheptan-1-one 935264-40-7P 935264-41-8P, Methyl 2-[2-(7-phenylheptanoyl)oxazol-5-yl]isonicotinate 935264-42-9P 935264-43-0P, 6-[2-(7-Phenylheptanoyl)oxazol-5-yl]picolinic acid methyl ester 935264-50-9P, Methyl 5-[2-(7-phenylheptanoyl)oxazol-5-yl]furan-2-carboxylate 935264-52-1P, Methyl 5-[2-(7-phenylheptanoyl)oxazol-5-yl]thiophene-2-carboxylate 935264-55-4P, 1-[5-(2,6-Dimethoxypyrimidin-4-yl)oxazol-2-yl]-7-phenylheptan-1-one 935264-56-5P, 1-[5-(2,4-Dimethoxypyrimidin-5-yl)oxazol-2-yl]-7-phenylheptan-1-one

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of keto-oxazole compds. as modulators of fatty acid amide hydrolase)

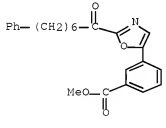
RN 935263-84-6 ZCAPLUS
CN Benzoic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



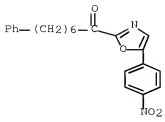
RN 935264-01-0 ZCAPLUS
CN 1-Heptanone, 1-[5-(3-nitrophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



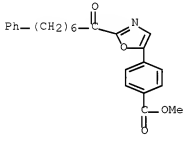
RN 935264-05-4 ZCAPLUS
CN Benzoic acid, 3-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



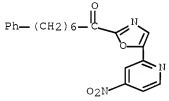
RN 935264-19-0 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-nitrophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



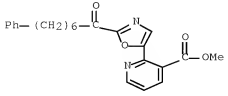
RN 935264-21-4 ZCAPLUS
CN Benzoic acid, 4-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



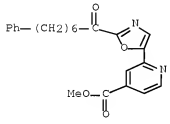
RN 935264-37-2 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-nitro-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



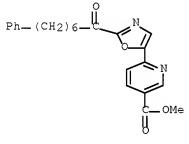
RN 935264-40-7 ZCAPLUS
CN 3-Pyridinecarboxylic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



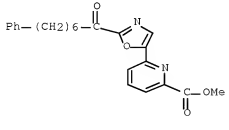
RN 935264-41-8 ZCAPLUS
CN 4-Pyridinecarboxylic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



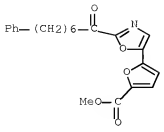
RN 935264-42-9 ZCAPLUS
CN 3-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



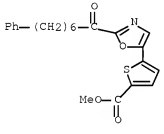
RN 935264-43-0 ZCAPLUS
CN 2-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



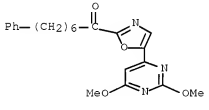
RN 935264-50-9 ZCAPLUS
CN 2-Furancarboxylic acid, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



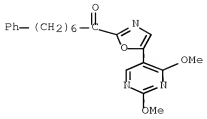
RN 935264-52-1 ZCAPLUS
CN 2-Thiophenecarboxylic acid, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



RN 935264-55-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(2,6-dimethoxy-4-pyrimidinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



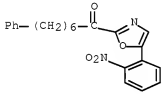
RN 935264-56-5 ZCAPLUS
CN 1-Heptanone, 1-[5-(2,4-dimethoxy-5-pyrimidinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



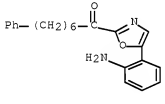
IT 935263-82-4P, 1-[5-(2-Nitrophenyl)oxazol-2-yl]-7-phenylheptan-1-one 935263-83-5P, 1-[5-(2-Aminophenyl)oxazol-2-yl]-7-phenylheptan-1-one 935263-85-7P, 2-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzoic acid 935263-87-9P, 1-[5-(2-Fluorophenyl)oxazol-2-yl]-7-phenylheptan-1-one 935263-89-1P, 1-[5-(2-Methoxyphenyl)oxazol-2-yl]-7-phenylheptan-1-one 935263-91-5P, 1-[5-(2-Hydroxyphenyl)oxazol-2-yl]-7-phenylheptan-1-one 935263-93-7P, 2-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzenesulfonamide 935263-95-9P, 2-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzamide 935263-97-1P, 7-Phenyl-1-[5-[2-(2,2,2-trifluoroacetyl)phenyl]oxazol-2-yl]heptan-1-one 935263-99-3P, 2-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzonitrile 935264-03-2P, 1-[5-(3-Aminophenyl)oxazol-2-yl]-7-phenylheptan-1-one 935264-07-6P, 3-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzoic acid 935264-09-8P, 1-[5-(3-Fluorophenyl)oxazol-2-yl]-7-phenylheptan-1-one 935264-11-2P, 1-[5-(3-Methoxyphenyl)oxazol-2-yl]-7-phenylheptan-1-one 935264-13-4P, 1-[5-(3-Hydroxyphenyl)oxazol-2-yl]-7-phenylheptan-1-one 935264-15-6P, 3-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzenesulfonamide 935264-16-7P, 3-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzamide 935264-17-8P, 7-Phenyl-1-[5-[3-(2,2,2-trifluoroacetyl)phenyl]oxazol-2-yl]heptan-1-one 935264-18-9P, 3-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzonitrile 935264-20-3P, 1-[5-(4-Aminophenyl)oxazol-2-yl]-7-phenylheptan-1-one 935264-22-5P , 4-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzoic acid 935264-23-6P, 1-[5-(4-Fluorophenyl)oxazol-2-yl]-7-phenylheptan-1-one 935264-24-7P, 1-[5-(4-Methoxyphenyl)oxazol-2-yl]-7-phenylheptan-1-one 935264-25-8P, 1-[5-(4-Hydroxyphenyl)oxazol-2-yl]-7-phenylheptan-1-one 935264-26-9P, 4-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzenesulfonamide 935264-27-0P, 4-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzamide 935264-28-1P, 7-Phenyl-1-[5-[4-(2,2,2-trifluoroacetyl)phenyl]oxazol-2-yl]heptan-1-one 935264-29-2P, 4-[2-(7-Phenylheptanoyl)oxazol-5-yl]benzonitrile 935264-30-5P, 1-[5-(3-Methylpyridin-2-yl)oxazol-2-yl]-7-phenylheptan-1-one 935264-31-6P, 1-[5-(4-Methylpyridin-2-yl)oxazol-2-yl]-7-phenylheptan-1-one 935264-32-7P, 1-[5-(5-Methylpyridin-2-yl)oxazol-2-yl]-7-phenylheptan-1-one 935264-33-8P, 1-[5-(6-Methylpyridin-2-yl)oxazol-2-yl]-7-phenylheptan-1-one 935264-34-9P, 1-[5-(4-Methoxypyridin-2-yl)oxazol-2-yl]-7-phenylheptan-1-one 935264-35-0P, 2-[2-(7-Phenylheptanoyl)oxazol-5-yl]isonicotinonitrile 935264-36-1P, 7-Phenyl-1-[5-[4-(trifluoromethyl)pyridin-2-yl]oxazol-2-yl]heptan-1-one 935264-38-3P, 1-[5-(4-Aminopyridin-2-yl)oxazol-2-yl]-7-phenylheptan-1-one 935264-39-4P, 1-[5-(4-Fluoropyridin-2-yl)oxazol-2-yl]-7-phenylheptan-1-one 935264-44-1P, 2-[2-(7-Phenylheptanoyl)oxazol-5-yl]nicotinic acid 935264-45-2P, 2-[2-(7-Phenylheptanoyl)oxazol-5-yl]isonicotinic

acid 935264-51-0P, 5-[2-(7-Phenylheptanoyl)oxazol-5-yl]furan-2-carboxylic acid 935264-53-2P, 5-[2-(7-Phenylheptanoyl)oxazol-5-yl]thiophene-2-carboxylic acid 935264-54-3P, 5-[2-(7-Phenylheptanoyl)oxazol-5-yl]thiophene-2-sulfonamide 935264-85-0P, 6-[2-(7-Phenylheptanoyl)oxazol-5-yl]pyrimidine-2,4(1H,3H)-dione 935264-87-2P, 5-[2-(7-Phenylheptanoyl)oxazol-5-yl]pyrimidine-2,4(1H,3H)-dione 947668-69-1P, 1-[5-(1-Methyl-1H-imidazol-2-yl)oxazol-2-yl]-7-phenylheptan-1-one 947668-70-4P, 1-[5-(1-Methyl-1H-tetrazol-5-yl)oxazol-2-yl]-7-phenylheptan-1-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of keto-oxazole compds. as modulators of fatty acid amide hydrolase)

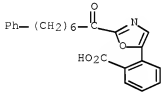
RN 935263-82-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-nitrophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



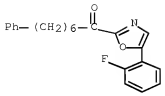
RN 935263-83-5 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-aminophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



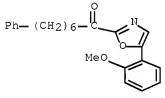
RN 935263-85-7 ZCAPLUS
CN Benzoic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



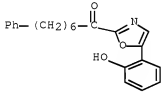
RN 935263-87-9 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-fluorophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



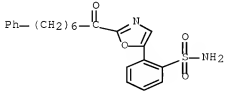
RN 935263-89-1 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-methoxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



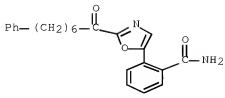
RN 935263-91-5 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-hydroxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



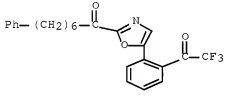
RN 935263-93-7 ZCAPLUS
CN Benzenesulfonamide, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



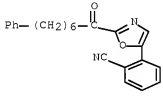
RN 935263-95-9 ZCAPLUS
CN Benzamide, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



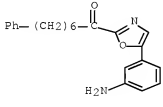
RN 935263-97-1 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-[2-(2,2,2-trifluoroacetyl)phenyl]-2-oxazolyl]-
(CA INDEX NAME)



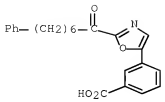
RN 935263-99-3 ZCAPLUS
CN Benzonitrile, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



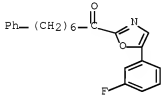
RN 935264-03-2 ZCAPLUS
CN 1-Heptanone, 1-[5-(3-aminophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



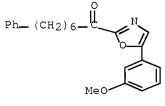
RN 935264-07-6 ZCAPLUS
CN Benzoic acid, 3-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



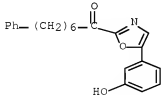
RN 935264-09-8 ZCAPLUS
CN 1-Heptanone, 1-[5-(3-fluorophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



RN 935264-11-2 ZCAPLUS
CN 1-Heptanone, 1-[5-(3-methoxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)

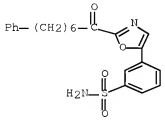


RN 935264-13-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(3-hydroxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)

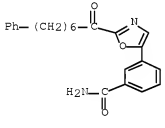


RN 935264-15-6 ZCAPLUS

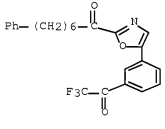
CN Benzenesulfonamide, 3-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



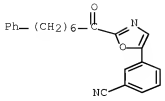
RN 935264-16-7 ZCAPLUS
CN Benzamide, 3-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



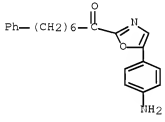
RN 935264-17-8 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-[3-(2,2,2-trifluoroacetyl)phenyl]-2-oxazolyl]- (CA INDEX NAME)



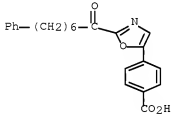
RN 935264-18-9 ZCAPLUS
CN Benzonitrile, 3-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



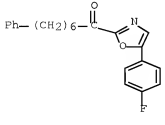
RN 935264-20-3 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-aminophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



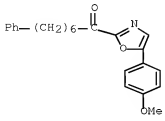
RN 935264-22-5 ZCAPLUS
CN Benzoic acid, 4-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



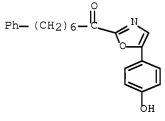
RN 935264-23-6 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-fluorophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



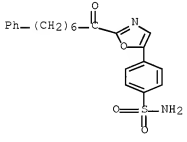
RN 935264-24-7 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-methoxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



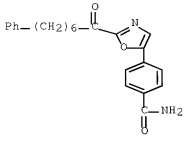
RN 935264-25-8 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-hydroxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



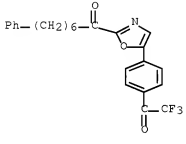
RN 935264-26-9 ZCAPLUS
CN Benzenesulfonamide, 4-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



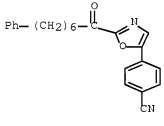
RN 935264-27-0 ZCAPLUS
CN Benzamide, 4-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



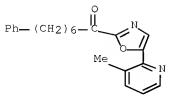
RN 935264-28-1 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-[4-(2,2,2-trifluoroacetyl)phenyl]-2-oxazolyl]- (CA INDEX NAME)



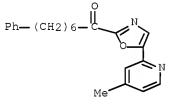
RN 935264-29-2 ZCAPLUS
CN Benzonitrile, 4-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



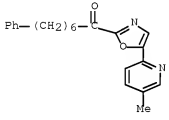
RN 935264-30-5 ZCAPLUS
CN 1-Heptanone, 1-[5-(3-methyl-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



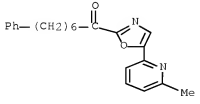
RN 935264-31-6 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-methyl-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



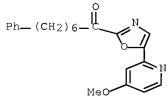
RN 935264-32-7 ZCAPLUS
CN 1-Heptanone, 1-[5-(5-methyl-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



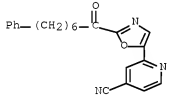
RN 935264-33-8 ZCAPLUS
CN 1-Heptanone, 1-[5-(6-methyl-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



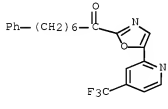
RN 935264-34-9 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-methoxy-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



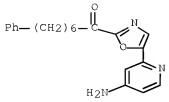
RN 935264-35-0 ZCAPLUS
CN 4-Pyridinecarbonitrile, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



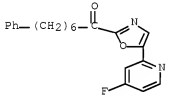
RN 935264-36-1 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-[4-(trifluoromethyl)-2-pyridinyl]-2-oxazolyl]- (CA INDEX NAME)



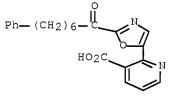
RN 935264-38-3 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-amino-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



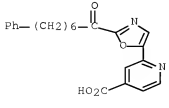
RN 935264-39-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-fluoro-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



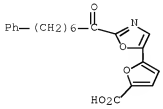
RN 935264-44-1 ZCAPLUS
CN 3-Pyridinecarboxylic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



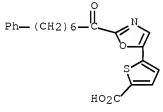
RN 935264-45-2 ZCAPLUS
CN 4-Pyridinecarboxylic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



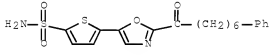
RN 935264-51-0 ZCAPLUS
CN 2-Furancarboxylic acid, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



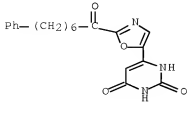
RN 935264-53-2 ZCAPLUS
CN 2-Thiophenecarboxylic acid, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



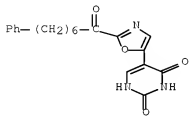
RN 935264-54-3 ZCAPLUS
CN 2-Thiophenesulfonamide, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



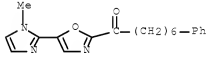
RN 935264-85-0 ZCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



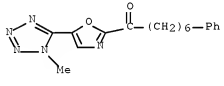
RN 935264-87-2 ZCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



RN 947668-69-1 ZCAPLUS
CN 1-Heptanone, 1-[5-(1-methyl-1H-imidazol-2-yl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)

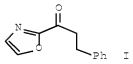


RN 947668-70-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(1-methyl-1H-tetrazol-5-yl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



L31 ANSWER 8 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:678848 ZCAPLUS Full-text
DOCUMENT NUMBER: 147:277494
TITLE: Reactions between Weinreb Amides and 2-Magnesiated Oxazoles: A Simple and Efficient Preparation of 2-Acyl Oxazoles
AUTHOR(S): Pippel, Daniel J.; Mapes, Christopher M.; Mani, Neelakandha S.
CORPORATE SOURCE: Johnson & Johnson Pharmaceutical Research and Development L.L.C., San Diego, CA, 92121, USA
SOURCE: Journal of Organic Chemistry (2007), 72(15), 5828-5831

CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:277494
GI

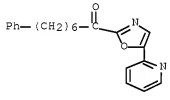


I

AB Treatment of oxazole or 5-aryloxazoles with i-PrMgCl smoothly generates the corresponding 2-Grignard reagents, which react with Weinreb amides to provide exclusively 2-acyloxazole products. E.g., reaction of oxazole with i-PrMgCl followed by reaction with PhCH2CH2CONMeOMe gave 76% acyloxazole I.

IT 681135-77-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-acyloxazoles by reaction of oxazole or 5-aryl oxazoles with i-PrMgCl followed by reaction with Weinreb amides)

RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

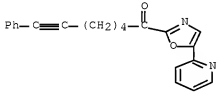
L31 ANSWER 9 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:626893 ZCAPLUS Full-text
DOCUMENT NUMBER: 147:229286
TITLE: Structure-Activity Relationships of α-Ketooxazole Inhibitors of Fatty Acid Amide Hydrolase
AUTHOR(S): Hardouin, Christophe; Kelso, Michael J.; Romero, F. Anthony; Rayl, Thomas J.; Leung, Donmienne; Hwang, Inkyu; Cravatt, Benjamin F.; Boger, Dale L.
CORPORATE SOURCE: Departments of Chemistry and Cell Biology and The Skaggs Institute for Chemical Biology, Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of Medicinal Chemistry (2007), 50(14), 3359-3368
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:229286

AB A systematic study of the structure-activity relationships of 2b (OL-135), a potent inhibitor of fatty acid amide hydrolase (FAAH), is detailed targeting the C2 acyl side chain. A series of aryl replacements or substituents for the terminal Ph group provided effective inhibitors (e.g., 5c, aryl = 1-naphthyl, Ki = 2.6 nM), with 5hh (aryl = 3-ClPh, Ki = 900 pM) being 5-fold more potent than 2b. Conformationally restricted C2 side chains were examined, and many provided exceptionally potent inhibitors, of which 11j (ethylbiphenyl side chain) was established to be a 750 pM inhibitor. A systematic series of heteroatoms (O, NMe, S), electron-withdrawing groups (SO, SO2), and amides positioned within and hydroxyl substitutions on the linking side chain were investigated, which typically led to a loss in potency. The most tolerant positions provided effective inhibitors (12p, 6-position S, Ki = 3 nM, or 13d, 2-position OH, Ki = 8 nM) comparable in potency to 2b. Proteome-wide screening of selected inhibitors from the systematic series of >100 candidates prepared revealed that they are selective for FAAH over all other mammalian serine proteases.

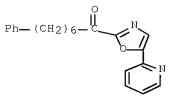
IT 808134-54-5
RL: PAC (Pharmacological activity); BIOL (Biological study)
(structure-activity relationships of ketooxazole inhibitors of fatty acid amide hydrolase)

RN 808134-54-5 ZCAPLUS
CN 6-Heptyn-1-one, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

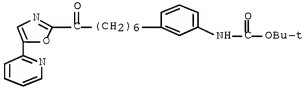


IT 681135-77-3P 945413-19-4P 945413-20-7P
945413-24-1P 945413-25-2P 945413-26-3P
945413-31-0P 945413-32-1P 945413-33-2P
945413-46-7P 945413-47-8P 945413-48-9P
945413-50-3P 945413-51-4P 945413-52-5P
945413-53-6P 945413-54-7P 945413-55-8P
945413-56-9P 945413-57-0P 945413-58-1P
945413-59-2P 945413-60-5P 945413-61-6P
945413-62-7P 945413-63-8P 945413-64-9P
945413-65-0P 945413-99-0P 945414-00-6P
945414-07-3P 945414-08-4P 945414-20-0P
945414-44-8P 945414-47-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(structure-activity relationships of ketooxazole inhibitors of fatty acid amide hydrolase)

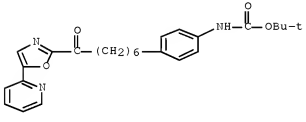
RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



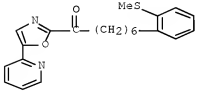
RN 945413-19-4 ZCAPLUS
CN Carbamic acid, N-[3-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]heptyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 945413-20-7 ZCAPLUS
CN Carbamic acid, N-[4-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]heptyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

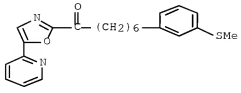


RN 945413-24-1 ZCAPLUS
CN 1-Heptanone, 7-[2-(methylthio)phenyl]-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

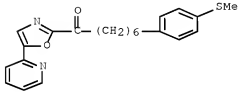


RN 945413-25-2 ZCAPLUS

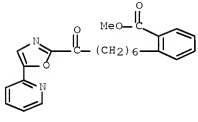
CN 1-Heptanone, 7-[3-(methylthio)phenyl]-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



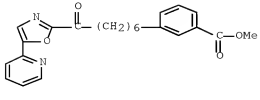
RN 945413-26-3 ZCAPLUS
CN 1-Heptanone, 7-[4-(methylthio)phenyl]-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



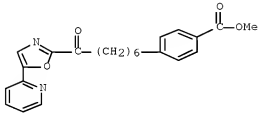
RN 945413-31-0 ZCAPLUS
CN Benzoic acid, 2-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]heptyl]-, methyl ester (CA INDEX NAME)



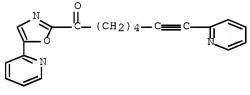
RN 945413-32-1 ZCAPLUS
CN Benzoic acid, 3-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]heptyl]-, methyl ester (CA INDEX NAME)



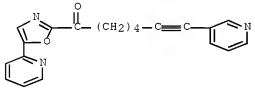
RN 945413-33-2 ZCAPLUS
CN Benzoic acid, 4-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]heptyl]-, methyl ester (CA INDEX NAME)



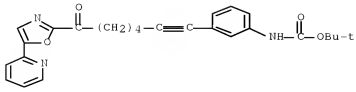
RN 945413-46-7 ZCAPLUS
CN 6-Heptyn-1-one, 7-(2-pyridinyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



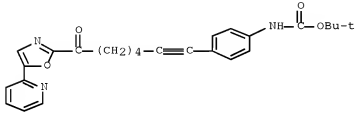
RN 945413-47-8 ZCAPLUS
CN 6-Heptyn-1-one, 7-(3-pyridinyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



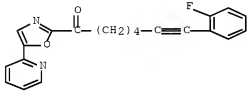
RN 945413-48-9 ZCAPLUS
CN Carbamic acid, N-[3-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]-1-heptyn-1-yl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



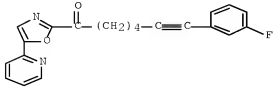
RN 945413-50-3 ZCAPLUS
CN Carbamic acid, N-[4-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]-1-heptyn-1-yl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 945413-51-4 ZCAPLUS
CN 6-Heptyn-1-one, 7-(2-fluorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

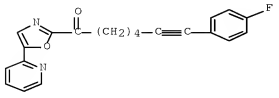


RN 945413-52-5 ZCAPLUS
CN 6-Heptyn-1-one, 7-(3-fluorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

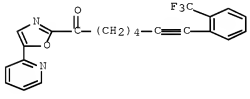


RN 945413-53-6 ZCAPLUS

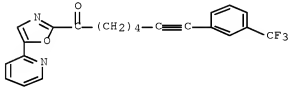
CN 6-Heptyn-1-one, 7-(4-fluorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



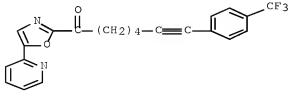
RN 945413-54-7 ZCAPLUS
CN 6-Heptyn-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]-7-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)



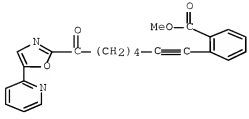
RN 945413-55-8 ZCAPLUS
CN 6-Heptyn-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]-7-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



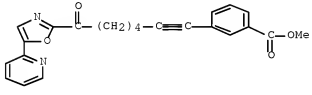
RN 945413-56-9 ZCAPLUS
CN 6-Heptyn-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]-7-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



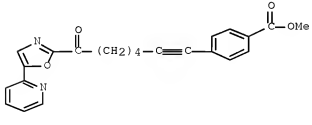
RN 945413-57-0 ZCAPLUS
CN Benzoic acid, 2-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]-1-heptyn-1-yl]-, methyl ester (CA INDEX NAME)



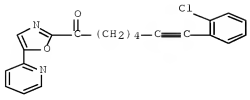
RN 945413-58-1 ZCAPLUS
CN Benzoic acid, 3-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]-1-heptyn-1-yl]-, methyl ester (CA INDEX NAME)



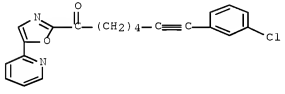
RN 945413-59-2 ZCAPLUS
CN Benzoic acid, 4-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]-1-heptyn-1-yl]-, methyl ester (CA INDEX NAME)



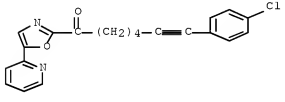
RN 945413-60-5 ZCAPLUS
CN 6-Heptyn-1-one, 7-(2-chlorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



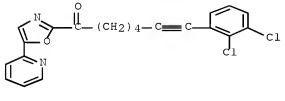
RN 945413-61-6 ZCAPLUS
CN 6-Heptyn-1-one, 7-(3-chlorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



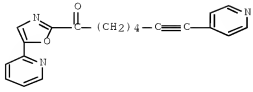
RN 945413-62-7 ZCAPLUS
CN 6-Heptyn-1-one, 7-(4-chlorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



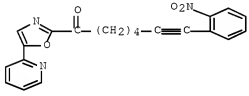
RN 945413-63-8 ZCAPLUS
CN 6-Heptyn-1-one, 7-(2,3-dichlorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



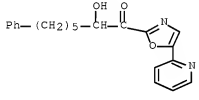
RN 945413-64-9 ZCAPLUS
CN 6-Heptyn-1-one, 7-(4-pyridinyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



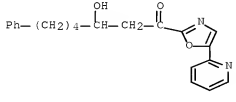
RN 945413-65-0 ZCAPLUS
CN 6-Heptyn-1-one, 7-(2-nitrophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



RN 945413-99-0 ZCAPLUS
CN 1-Heptanone, 2-hydroxy-7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

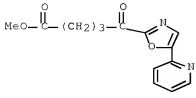


RN 945414-00-6 ZCAPLUS
CN 1-Heptanone, 3-hydroxy-7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



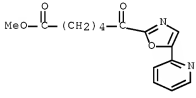
RN 945414-07-3 ZCAPLUS

CN 2-Oxazolepentanoic acid, δ-oxo-5-(2-pyridinyl)-, methyl ester (CA INDEX NAME)



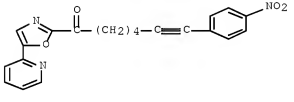
RN 945414-08-4 ZCAPLUS

CN 2-Oxazolehexanoic acid, ε-oxo-5-(2-pyridinyl)-, methyl ester (CA INDEX NAME)



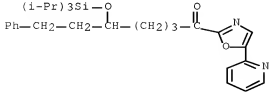
RN 945414-20-0 ZCAPLUS

CN 6-Heptyn-1-one, 7-(4-nitrophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

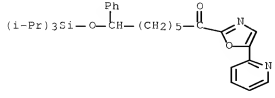


RN 945414-44-8 ZCAPLUS

CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]-5-[[tris(1-methylethyl)silyl]oxy]- (CA INDEX NAME)

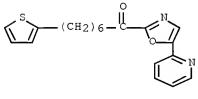


RN 945414-47-1 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]-7-[[tris(1-methylethyl)silyl]oxy]- (CA INDEX NAME)

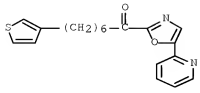


IT 945413-05-8P 945413-06-9P 945413-07-0P
945413-08-1P 945413-09-2P 945413-10-5P
945413-11-6P 945413-12-7P 945413-13-8P
945413-14-9P 945413-15-0P 945413-16-1P
945413-17-2P 945413-18-3P 945413-21-8P
945413-22-9P 945413-23-0P 945413-27-4P
945413-28-5P 945413-29-6P 945413-30-9P
945413-34-3P 945413-35-4P 945413-36-5P
945413-37-6P 945413-38-7P 945413-39-8P
945413-40-1P 945413-41-2P 945413-42-3P
945413-43-4P 945413-44-5P 945413-45-6P
945413-66-1P 945413-89-8P 945413-90-1P
945413-94-5P 945413-95-6P 945413-97-8P
945413-98-9P 945414-02-8P 945414-03-9P
945414-04-0P 945414-05-1P 945414-12-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(structure-activity relationships of ketooxazole inhibitors of fatty acid amide hydrolase)

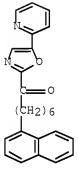
RN 945413-05-8 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-pyridinyl)-2-oxazolyl]-7-(2-thienyl)- (CA INDEX NAME)



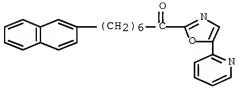
RN 945413-06-9 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-pyridinyl)-2-oxazolyl]-7-(3-thienyl)- (CA INDEX NAME)



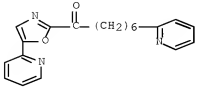
RN 945413-07-0 ZCAPLUS
CN 1-Heptanone, 7-(1-naphthalenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



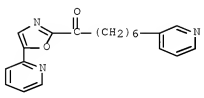
RN 945413-08-1 ZCAPLUS
CN 1-Heptanone, 7-(2-naphthalenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



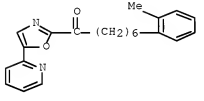
RN 945413-09-2 ZCAPLUS
CN 1-Heptanone, 7-(2-pyridinyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



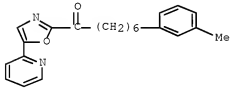
RN 945413-10-5 ZCAPLUS
CN 1-Heptanone, 7-(3-pyridinyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



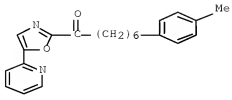
RN 945413-11-6 ZCAPLUS
CN 1-Heptanone, 7-(2-methylphenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



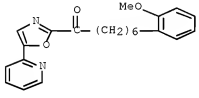
RN 945413-12-7 ZCAPLUS
CN 1-Heptanone, 7-(3-methylphenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



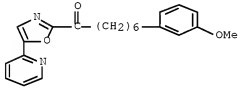
RN 945413-13-8 ZCAPLUS
CN 1-Heptanone, 7-(4-methylphenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



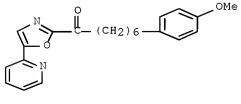
RN 945413-14-9 ZCAPLUS
CN 1-Heptanone, 7-(2-methoxyphenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



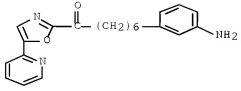
RN 945413-15-0 ZCAPLUS
CN 1-Heptanone, 7-(3-methoxyphenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



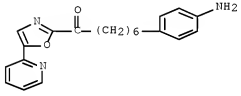
RN 945413-16-1 ZCAPLUS
CN 1-Heptanone, 7-(4-methoxyphenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



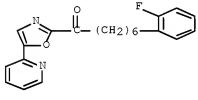
RN 945413-17-2 ZCAPLUS
CN 1-Heptanone, 7-(3-aminophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



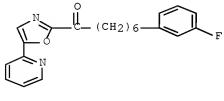
RN 945413-18-3 ZCAPLUS
CN 1-Heptanone, 7-(4-aminophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



RN 945413-21-8 ZCAPLUS
CN 1-Heptanone, 7-(2-fluorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

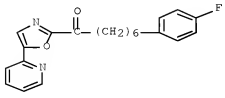


RN 945413-22-9 ZCAPLUS
CN 1-Heptanone, 7-(3-fluorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

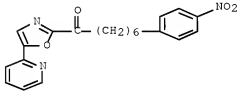


RN 945413-23-0 ZCAPLUS

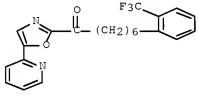
CN 1-Heptanone, 7-(4-fluorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



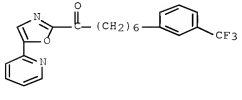
RN 945413-27-4 ZCAPLUS
CN 1-Heptanone, 7-(4-nitrophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



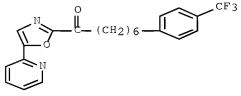
RN 945413-28-5 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-pyridinyl)-2-oxazolyl]-7-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)



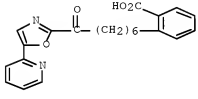
RN 945413-29-6 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-pyridinyl)-2-oxazolyl]-7-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



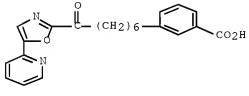
RN 945413-30-9 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-pyridinyl)-2-oxazolyl]-7-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



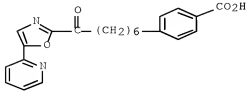
RN 945413-34-3 ZCAPLUS
CN Benzoic acid, 2-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]heptyl]- (CA INDEX NAME)



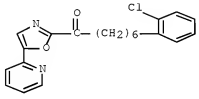
RN 945413-35-4 ZCAPLUS
CN Benzoic acid, 3-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]heptyl]- (CA INDEX NAME)



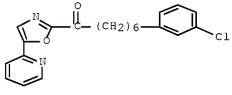
RN 945413-36-5 ZCAPLUS
CN Benzoic acid, 4-[7-oxo-7-[5-(2-pyridinyl)-2-oxazolyl]heptyl]- (CA INDEX NAME)



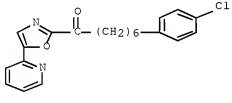
RN 945413-37-6 ZCAPLUS
CN 1-Heptanone, 7-(2-chlorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



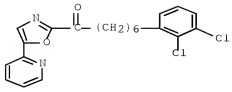
RN 945413-38-7 ZCAPLUS
CN 1-Heptanone, 7-(3-chlorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



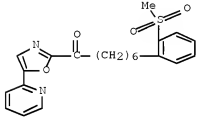
RN 945413-39-8 ZCAPLUS
CN 1-Heptanone, 7-(4-chlorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



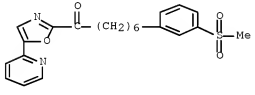
RN 945413-40-1 ZCAPLUS
CN 1-Heptanone, 7-(2,3-dichlorophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



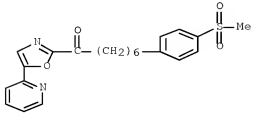
RN 945413-41-2 ZCAPLUS
CN 1-Heptanone, 7-[2-(methylsulfonyl)phenyl]-1-[5-(2-pyridinyl)-2-oxazolyl]-
(CA INDEX NAME)



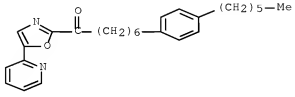
RN 945413-42-3 ZCAPLUS
CN 1-Heptanone, 7-[3-(methylsulfonyl)phenyl]-1-[5-(2-pyridinyl)-2-oxazolyl]-
(CA INDEX NAME)



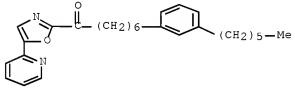
RN 945413-43-4 ZCAPLUS
CN 1-Heptanone, 7-[4-(methylsulfonyl)phenyl]-1-[5-(2-pyridinyl)-2-oxazolyl]-
(CA INDEX NAME)



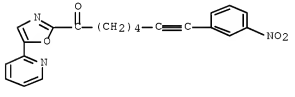
RN 945413-44-5 ZCAPLUS
CN 1-Heptanone, 7-(4-hexylphenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



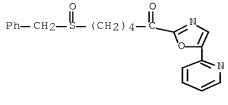
RN 945413-45-6 ZCAPLUS
CN 1-Heptanone, 7-(3-hexylphenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



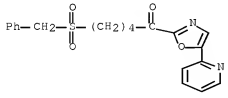
RN 945413-66-1 ZCAPLUS
CN 6-Heptyn-1-one, 7-(3-nitrophenyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



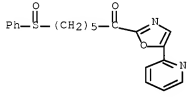
RN 945413-89-8 ZCAPLUS
CN 1-Pentanone, 5-[(phenylmethyl)sulfinyl]-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



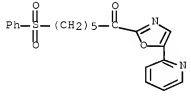
RN 945413-90-1 ZCAPLUS
CN 1-Pentanone, 5-[(phenylmethyl)sulfonyl]-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



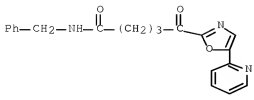
RN 945413-94-5 ZCAPLUS
CN 1-Hexanone, 6-(phenylsulfinyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



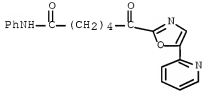
RN 945413-95-6 ZCAPLUS
CN 1-Hexanone, 6-(phenylsulfonyl)-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



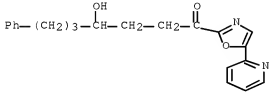
RN 945413-97-8 ZCAPLUS
CN 2-Oxazolepentanamide, δ-oxo-N-(phenylmethyl)-5-(2-pyridinyl)- (CA INDEX NAME)



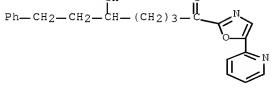
RN 945413-98-9 ZCAPLUS
CN 2-Oxazolehexanamide, ε-oxo-N-phenyl-5-(2-pyridinyl)- (CA INDEX NAME)



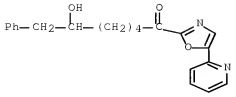
RN 945414-02-8 ZCAPLUS
CN 1-Heptanone, 4-hydroxy-7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



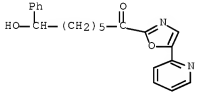
RN 945414-03-9 ZCAPLUS
CN 1-Heptanone, 5-hydroxy-7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



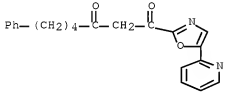
RN 945414-04-0 ZCAPLUS
CN 1-Heptanone, 6-hydroxy-7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



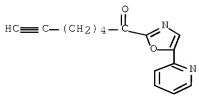
RN 945414-05-1 ZCAPLUS
CN 1-Heptanone, 7-hydroxy-7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



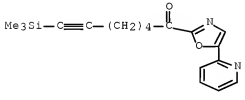
RN 945414-12-0 ZCAPLUS
CN 1,3-Heptanedione, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



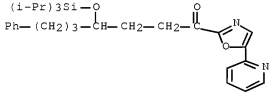
IT 808134-52-3P 808134-53-4P 945414-73-3P
945414-86-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(structure-activity relationships of ketooxazole inhibitors of fatty acid amide hydrolase)
RN 808134-52-3 ZCAPLUS
CN 6-Heptyn-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



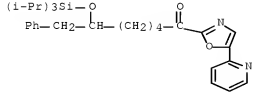
RN 808134-53-4 ZCAPLUS
CN 6-Heptyn-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]-7-(trimethylsilyl)- (CA INDEX NAME)



RN 945414-73-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]-4-[[tris(1-methylethyl)silyl]oxy]- (CA INDEX NAME)



RN 945414-86-8 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]-6-[[tris(1-methylethyl)silyl]oxy]- (CA INDEX NAME)



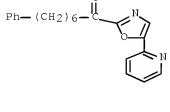
REFERENCE COUNT: 88 THERE ARE 88 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 10 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:471316 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:475484
TITLE: Evaluation of fatty acid amide hydrolase inhibition in murine models of emotionality
AUTHOR(S): Naidu, Pattipati S.; Varvel, Stephen A.; Ahn, Kyunghye; Cravatt, Benjamin F.; Martin, Billy R.; Lichtman, Aron H.
CORPORATE SOURCE: Department of Pharmacology and Toxicology, Medical College of Virginia Campus, Virginia Commonwealth University, Richmond, VA, 23298-0613, USA
SOURCE: Psychopharmacology (Berlin, Germany) (2007), 192(1), 61-70
CODEN: PSCHDL; ISSN: 0033-3158
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Rationale: Manipulations of the endocannabinoid/fatty acid amide hydrolase (FAAH) signaling systems result in conflicting and paradoxical effects in rodent models of emotional reactivity. Objectives: In the present study, we tested the hypothesis that the inhibition of FAAH would elicit significant effects in murine models used to screen anxiolytic and antidepressant drugs. Materials and methods: FAAH (-/-) mice and wild-type mice treated with FAAH inhibitors (URB597 and OL-135) were evaluated in standard behavioral screening models for antidepressant (i.e., tail suspension and forced-swim tests) and anxiolytic (i.e., elevated plus maze) agents. The doses of URB597 and OL-135 selected were based on their ability to augment the pharmacol. effects (i.e., analgesia, catalepsy, and hypothermia) of exogenously administered anandamide. Results: FAAH (-/-) mice, anandamide-injected FAAH (-/-) mice, or wild-type mice injected with FAAH inhibitors or anandamide failed to exhibit significant effects in standard tests of emotional reactivity, although the antidepressant desipramine and the anxiolytic agent midazolam were active in the appropriate assays. FAAH- (-/-) and URB597-treated mice finally displayed significant effects in the tail suspension test when substantial methodol. changes were made (i.e., altered ambient light and increased sample sizes). Conclusions: Although FAAH suppression can elicit significant effects under some instances in which consequential procedural modifications are made, the present results indicate that the pharmacol. inhibition or genetic deletion of FAAH is ineffective in standard mouse models of emotional reactivity. It remains to be established whether the effects of FAAH inhibition in these modified tasks are predictive of their efficacy in treating emotional disorders.

IT 681135-77-3, OL-135
RL: PAC (Pharmacological activity); BIOL (Biological study)
(evaluation of fatty acid amide hydrolase inhibition in murine models of emotionality)

RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



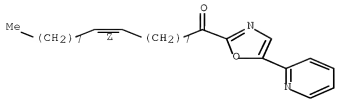
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 11 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:239663 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:455147
TITLE: Fatty acid amide hydrolase inhibitors display broad selectivity and inhibit multiple carboxylesterases as off-targets
AUTHOR(S): Zhang, Di; Saraf, Anita; Kolasa, Teodozyi; Bhatia, Pramila; Zheng, Guo Zhu; Patel, Meena; Lannoye, Greg S.; Richardson, Paul; Stewart, Andrew; Rogers, John C.; Brioni, Jorge D.; Surowy, Carol S.
CORPORATE SOURCE: Neuroscience Research, Advanced Technology and Process Research and Development, Global Pharmaceutical Research and Development, Abbott Laboratories, Abbott Park, IL, 60064, USA
SOURCE: Neuropharmacology (2007), 52(4), 1095-1105
CODEN: NEPHBW; ISSN: 0028-3908
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

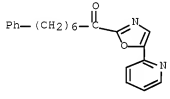
AB Fatty acid amide hydrolase (FAAH) is the primary regulator of several bioactive lipid amides including anandamide. Inhibitors of FAAH are potentially useful for the treatment of pain, anxiety, depression, and other nervous system disorders. However, FAAH inhibitors must display selectivity for this enzyme relative to the numerous other serine hydrolases present in the human proteome in order to be therapeutically acceptable. Here we employed activity-based protein profiling (ABPP) to assess the selectivity of FAAH inhibitors in multiple rat and human tissues. We discovered that some inhibitors, including carbamate compds. SA-47 and SA-72, and AM404 are exceptionally selective while others, like URB597, BMS-1, OL-135, and LY2077855 are less selective, displaying multiple off-targets. Since proteins around 60 kDa constitute the major off-targets for URB597 and several other FAAH inhibitors with different chemical structures, we employed the multi-dimensional protein identification technol. (MudPIT) approach to analyze their identities. We identified multiple carboxylesterase isoenzymes as bona fide off-targets of FAAH inhibitors. Consistently, enzymic assay confirmed inhibition of carboxylesterase activities in rat liver by FAAH inhibitors. Since carboxylesterases hydrolyze a variety of ester-containing drugs and prodrugs, we speculate that certain FAAH inhibitors, by inhibiting carboxylesterases, might have drug-drug interactions with other medicines if developed as therapeutic agents.

IT 639819-38-8, α-KH 7 681135-77-3, OL-135
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fatty acid amide hydrolase inhibitors display broad selectivity and inhibit multiple carboxylesterases as offtargets)
RN 639819-38-8 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

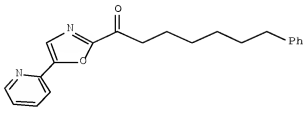


RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 12 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:128810 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:454140
TITLE: Potent and Selective α-Ketoheterocycle-Based Inhibitors of the Anandamide and Oleamide Catabolizing Enzyme, Fatty Acid Amide Hydrolase
AUTHOR(S): Romero, F. Anthony; Du, Wu; Hwang, Inkyu; Rayl, Thomas J.; Kimball, F. Scott; Leung, Donmienne; Hoover, Heather S.; Apodaca, Richard L.; Breitenbucher, J. Guy; Cravatt, Benjamin F.; Boger, Dale L.
CORPORATE SOURCE: Departments of Chemistry Cell Biology and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of Medicinal Chemistry (2007), 50(5), 1058-1068
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:454140
GI



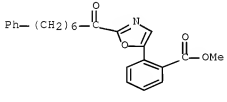
I

AB A study of the structure-activity relationships (SAR) of 2f (I, OL-135), a potent inhibitor of fatty acid amide hydrolase (FAAH), is detailed, targeting the 5-position of the oxazole. Examination of a series of substituted benzene derivs. (12-14) revealed that the optimal position for substitution was the meta-position with selected members approaching or exceeding the potency of 2f. Concurrent with these studies, the effect of substitution on the pyridine ring of 2f was also examined A series of small, nonarom. C5-substituents was also explored and revealed that the Ki follows a well-defined correlation with the Hammett σp constant (ρ = 3.01, R2 = 0.91) in which electron-withdrawing substituents enhance potency, leading to inhibitors with Kis as low as 400 pM (20n). Proteomic-wide screening of the inhibitors revealed that most are exquisitely selective for FAAH over all other mammalian proteases, reversing the 100-fold preference of 20a (C5 substituent = H) for the enzyme TGH.

IT 935263-84-6P 935264-01-0P 935264-05-4P
935264-13-0P 935264-37-2P 935264-40-7P
935264-41-8P 935264-42-9P 935264-43-0P
935264-55-4P 935264-56-5P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(keto heterocycle-based inhibitors of fatty acid amide hydrolase)

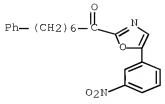
RN 935263-84-6 ZCAPLUS

CN Benzoic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)

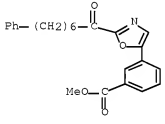


RN 935264-01-0 ZCAPLUS

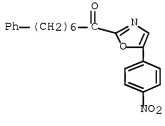
CN 1-Heptanone, 1-[5-(3-nitrophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



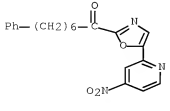
RN 935264-05-4 ZCAPLUS
CN Benzoic acid, 3-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



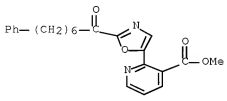
RN 935264-19-0 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-nitrophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



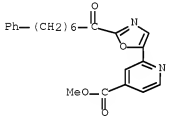
RN 935264-37-2 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-nitro-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



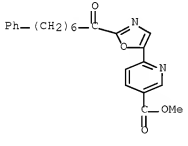
RN 935264-40-7 ZCAPLUS
CN 3-Pyridinecarboxylic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



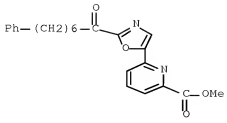
RN 935264-41-8 ZCAPLUS
CN 4-Pyridinecarboxylic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



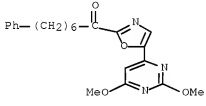
RN 935264-42-9 ZCAPLUS
CN 3-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



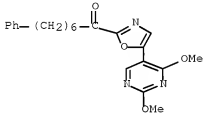
RN 935264-43-0 ZCAPLUS
CN 2-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



RN 935264-55-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(2,6-dimethoxy-4-pyrimidinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



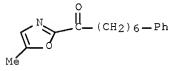
RN 935264-56-5 ZCAPLUS
CN 1-Heptanone, 1-[5-(2,4-dimethoxy-5-pyrimidinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



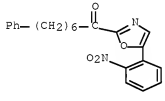
IT 914483-10-6P 935263-82-4P 935263-83-5P
935263-85-7P 935263-87-9P 935263-89-1P
935263-91-5P 935263-93-7P 935263-95-9P
935263-97-1P 935263-99-3P 935264-03-2P
935264-07-6P 935264-09-8P 935264-11-2P
935264-13-4P 935264-15-6P 935264-16-7P
935264-17-8P 935264-18-9P 935264-20-3P
935264-21-4P 935264-22-5P 935264-23-6P
935264-24-7P 935264-25-8P 935264-26-9P
935264-27-0P 935264-28-1P 935264-29-2P
935264-30-5P 935264-31-6P 935264-32-7P
935264-33-8P 935264-34-9P 935264-35-0P
935264-36-1P 935264-38-3P 935264-39-4P

935264-44-1P 935264-45-2P 935264-46-3P
935264-47-4P 935264-48-5P 935264-49-6P
935264-50-9P 935264-51-0P 935264-52-1P
935264-53-2P 935264-54-3P 935264-58-7P
935264-60-1P 935264-85-0P 935264-87-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(keto heterocycle-based inhibitors of fatty acid amide hydrolase)

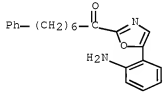
RN 914483-10-6 ZCAPLUS
CN 1-Heptanone, 1-(5-methyl-2-oxazolyl)-7-phenyl- (CA INDEX NAME)



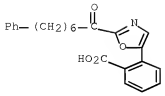
RN 935263-82-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-nitrophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



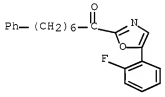
RN 935263-83-5 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-aminophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



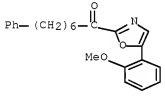
RN 935263-85-7 ZCAPLUS
CN Benzoic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



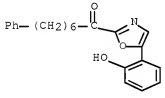
RN 935263-87-9 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-fluorophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



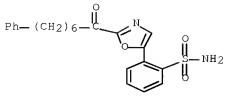
RN 935263-89-1 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-methoxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



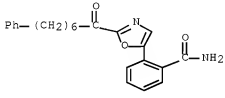
RN 935263-91-5 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-hydroxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



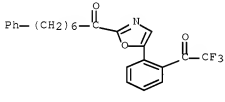
RN 935263-93-7 ZCAPLUS
CN Benzenesulfonamide, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



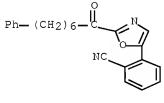
RN 935263-95-9 ZCAPLUS
CN Benzamide, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



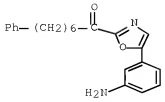
RN 935263-97-1 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-[2-(2,2,2-trifluoroacetyl)phenyl]-2-oxazolyl]-
(CA INDEX NAME)



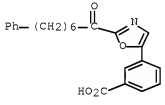
RN 935263-99-3 ZCAPLUS
CN Benzonitrile, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



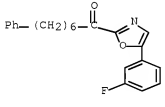
RN 935264-03-2 ZCAPLUS
CN 1-Heptanone, 1-[5-(3-aminophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



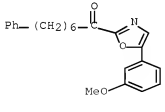
RN 935264-07-6 ZCAPLUS
CN Benzoic acid, 3-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



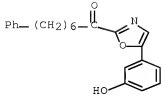
RN 935264-09-8 ZCAPLUS
CN 1-Heptanone, 1-[5-(3-fluorophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



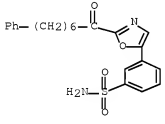
RN 935264-11-2 ZCAPLUS
CN 1-Heptanone, 1-[5-(3-methoxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



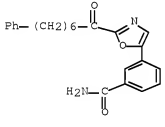
RN 935264-13-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(3-hydroxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



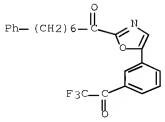
RN 935264-15-6 ZCAPLUS
CN Benzenesulfonamide, 3-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



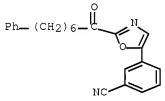
RN 935264-16-7 ZCAPLUS
CN Benzamide, 3-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



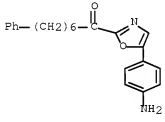
RN 935264-17-8 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-[3-(2,2,2-trifluoroacetyl)phenyl]-2-oxazolyl]- (CA INDEX NAME)



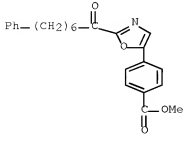
RN 935264-18-9 ZCAPLUS
CN Benzonitrile, 3-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



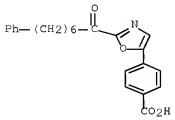
RN 935264-20-3 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-aminophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



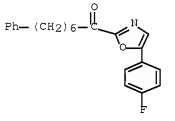
RN 935264-21-4 ZCAPLUS
CN Benzoic acid, 4-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



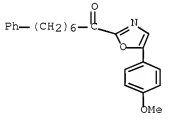
RN 935264-22-5 ZCAPLUS
CN Benzoic acid, 4-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



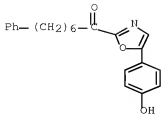
RN 935264-23-6 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-fluorophenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



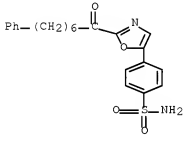
RN 935264-24-7 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-methoxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



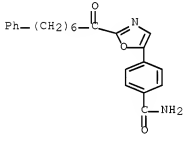
RN 935264-25-8 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-hydroxyphenyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



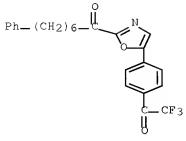
RN 935264-26-9 ZCAPLUS
CN Benzenesulfonamide, 4-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



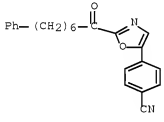
RN 935264-27-0 ZCAPLUS
CN Benzamide, 4-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



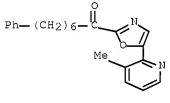
RN 935264-28-1 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-[4-(2,2,2-trifluoroacetyl)phenyl]-2-oxazolyl]- (CA INDEX NAME)



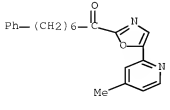
RN 935264-29-2 ZCAPLUS
CN Benzonitrile, 4-[2-(1-oxo-7-phenylhepty1)-5-oxazoly1]- (CA INDEX NAME)



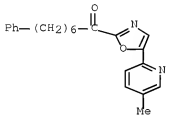
RN 935264-30-5 ZCAPLUS
CN 1-Heptanone, 1-[5-(3-methyl-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



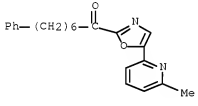
RN 935264-31-6 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-methyl-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



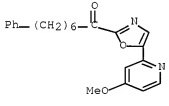
RN 935264-32-7 ZCAPLUS
CN 1-Heptanone, 1-[5-(5-methyl-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



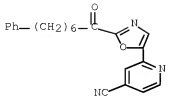
RN 935264-33-8 ZCAPLUS
CN 1-Heptanone, 1-[5-(6-methyl-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



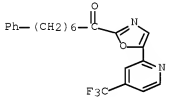
RN 935264-34-9 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-methoxy-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



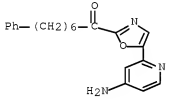
RN 935264-35-0 ZCAPLUS
CN 4-Pyridinecarbonitrile, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



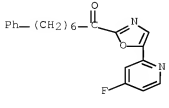
RN 935264-36-1 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-[4-(trifluoromethyl)-2-pyridinyl]-2-oxazolyl]- (CA INDEX NAME)



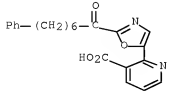
RN 935264-38-3 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-amino-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



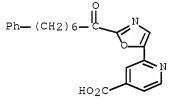
RN 935264-39-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(4-fluoro-2-pyridinyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



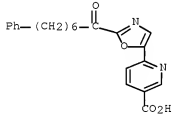
RN 935264-44-1 ZCAPLUS
CN 3-Pyridinecarboxylic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



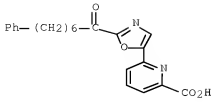
RN 935264-45-2 ZCAPLUS
CN 4-Pyridinecarboxylic acid, 2-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



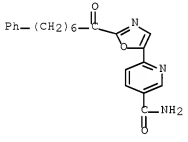
RN 935264-46-3 ZCAPLUS
CN 3-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



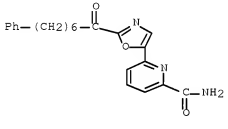
RN 935264-47-4 ZCAPLUS
CN 2-Pyridinecarboxylic acid, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



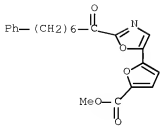
RN 935264-48-5 ZCAPLUS
CN 3-Pyridinecarboxamide, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



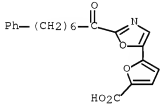
RN 935264-49-6 ZCAPLUS
CN 2-Pyridinecarboxamide, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



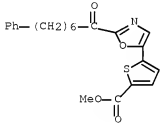
RN 935264-50-9 ZCAPLUS
CN 2-Furancarboxylic acid, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



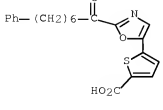
RN 935264-51-0 ZCAPLUS
CN 2-Furancarboxylic acid, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



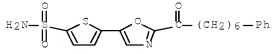
RN 935264-52-1 ZCAPLUS
CN 2-Thiophenecarboxylic acid, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]-, methyl ester (CA INDEX NAME)



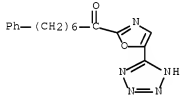
RN 935264-53-2 ZCAPLUS
CN 2-Thiophenecarboxylic acid, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



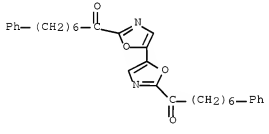
RN 935264-54-3 ZCAPLUS
CN 2-Thiophenesulfonamide, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



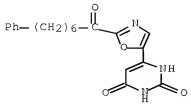
RN 935264-58-7 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2H-tetrazol-5-yl)-2-oxazolyl]- (CA INDEX NAME)



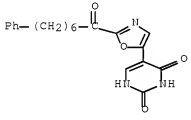
RN 935264-60-1 ZCAPLUS
CN 1-Heptanone, 1,1'-[5,5'-bioxazole]-2,2'-diylbis[7-phenyl- (CA INDEX NAME)



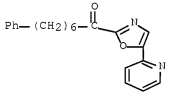
RN 935264-85-0 ZCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 6-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



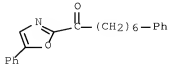
RN 935264-87-2 ZCAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 5-[2-(1-oxo-7-phenylheptyl)-5-oxazolyl]- (CA INDEX NAME)



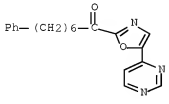
IT 681135-77-3, OL-135 808134-72-7 808134-74-9
808134-76-1 808134-77-2 808134-78-3
808134-79-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(keto heterocycle-based inhibitors of fatty acid amide hydrolase)
RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



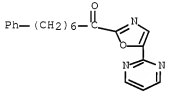
RN 808134-72-7 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-(5-phenyl-2-oxazolyl)- (CA INDEX NAME)



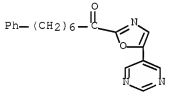
RN 808134-74-9 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(4-pyrimidinyl)-2-oxazolyl]- (CA INDEX NAME)



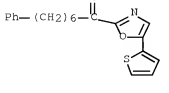
RN 808134-76-1 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyrimidinyl)-2-oxazolyl]- (CA INDEX NAME)



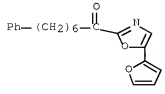
RN 808134-77-2 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(5-pyrimidinyl)-2-oxazolyl]- (CA INDEX NAME)



RN 808134-78-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-thienyl)-2-oxazolyl]- (CA INDEX NAME)

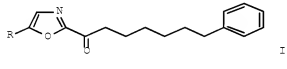


RN 808134-79-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-furanyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

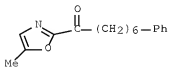
L31 ANSWER 13 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1058482 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:7854
TITLE: Delineation of a Fundamental α-Ketoheterocycle Substituent Effect for Use in the Design of Enzyme Inhibitors
AUTHOR(S): Romero, F. Anthony; Hwang, Inkyu; Boger, Dale L.
CORPORATE SOURCE: Department of Chemistry and the Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of the American Chemical Society (2006), 128(43), 14004-14005
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:7854
GI



I

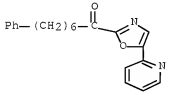
AB The synthesis and examination of a systematic series of 5-substituted α-ketooxazoles I (R = H, CO2H, CO2Me, CONH2, CONMe2, COMe, CHO, COCF3, CN, Me, CF3, I, Br, Cl, F, SMe) as inhibitors of fatty acid amide hydrolase (FAAH) defined a fundamental substituent effect that led to the discovery of inhibitors.
IT 914483-10-6P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, FAAH inhibition, and QSAR of phenylheptanoyloxazoles via lithiation of (t-butyldimethylsilyloxy)phenylheptyloxazole followed by addition to electrophiles, deprotection, and Dess-Martin oxidation)

RN 914483-10-6 ZCAPLUS
CN 1-Heptanone, 1-(5-methyl-2-oxazolyl)-7-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 14 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:399656 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:21002
TITLE: Inhibition of fatty acid amide hydrolase produces analgesia by multiple mechanisms. [Erratum to document cited in CA144:480898]
AUTHOR(S): Chang, Leon; Luo, Lin; Palmer, James A.; Sutton, Steven; Wilson, Sandy J.; Barbier, Ann J.; Breitenbucher, James Guy; Chaplan, Sandra R.; Webb, Michael
CORPORATE SOURCE: Johnson & Johnson Pharmaceutical Research & Development, L.L.C., San Diego, CA, 92121-1126, USA
SOURCE: British Journal of Pharmacology (2006), 148(1), 114
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English
AB On page 107, Figure 5 was published incorrectly. The correct figure and legend is given.
IT 681135-77-3, OL135
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of fatty acid amide hydrolase produces analgesia by multiple mechanisms (Erratum))
RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



L31 ANSWER 15 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:399647 ZCAPLUS Full-text
DOCUMENT NUMBER: 144:480898
TITLE: Inhibition of fatty acid amide hydrolase produces

analgesia by multiple mechanisms

AUTHOR(S): Chang, Leon; Luo, Lin; Palmer, James A.; Sutton, Steven; Wilson, Sandy J.; Barbier, Ann J.; Breitenbucher, James Guy; Chaplan, Sandra R.; Webb, Michael

CORPORATE SOURCE: Johnson & Johnson Pharmaceutical Research & Development, L.L.C., San Diego, CA, 92121-1126, USA

SOURCE: British Journal of Pharmacology (2006), 148(1), 102-113
CODEN: BJPCBM; ISSN: 0007-1188

PUBLISHER: Nature Publishing Group

DOCUMENT TYPE: Journal

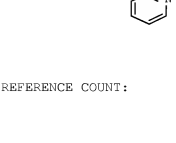
LANGUAGE: English

AB The reversible fatty acid amide hydrolase (FAAH) inhibitor OL135 reverses mech. allodynia in the spinal nerve ligation (SNL) and mild thermal injury (MTI) models in the rat. The purpose of this study was to investigate the role of the cannabinoid and opioid systems in mediating this analgesic effect. Elevated brain concns. of anandamide (350 pmol g-1 of tissue vs. 60 pmol g-1 in vehicle-treated controls) were found in brains of rats given OL135 (20 mg kg-1) i.p. 15 min prior to 20 mg kg-1 i.p. anandamide. Predosing rats with OL135 (2-60 mg kg-1 i.p.) 30 min before administration of an irreversible FAAH inhibitor (URB597: 0.3 mg kg-1 intracardiac) was found to protect brain FAAH from irreversible inactivation. The level of enzyme protection was correlated with the OL135 concns. in the same brains. OL135 (100 mg kg-1 i.p.) reduced by 50% of the maximum possible efficacy (MPE) mech. allodynia induced by MTI in FAAH+/+mice (von Frey filament measurement) 30 min after dosing, but was without effect in FAAH-/- mice. OL135 given i.p. resulted in a dose-responsive reversal of mech. allodynia in both MTI and SNL models in the rat with an ED50 between 6 and 9 mg kg-1. The plasma concentration at the ED50 in both models was 0.7 μM (240 ng ml-1). In the rat SNL model, coadministration of the selective CB2 receptor antagonist SR144528 (5 mg kg-1 i.p.), with 20 mg kg-1 OL135 blocked the OL135-induced reversal of mech. allodynia, but the selective CB1 antagonist SR141716A (5 mg kg-1 i.p.) was without effect. In the rat MTI model neither SR141716A or SR144528 (both at 5 mg kg-1 i.p.), or a combination of both antagonists coadministered with OL135 (20 mg kg-1) blocked reversal of mech. allodynia assessed 30 min after dosing. In both the MTI model and SNL models in rats, naloxone (1 mg kg-1, i.p. 30 min after OL135) reversed the analgesia (to 15% of control levels in the MTI model, to zero in the SNL) produced by OL135.

IT 681135-77-3, OL135
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of fatty acid amide hydrolase produces analgesia by multiple mechanisms)

RN 681135-77-3 ZCAPLUS

CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



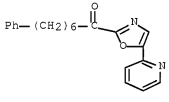
REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 16 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:148921 ZCAPLUS Full-text
DOCUMENT NUMBER: 144:205794
TITLE: Fatty acid amide hydrolase inhibitors for the treatment of neurodegenerative disease, and screening method
INVENTOR(S): Hillen, Heinz; Schmidt, Martin
PATENT ASSIGNEE(S): Abbott G.m.b.H. & Co. K.-G., Germany
SOURCE: Ger. Offen., 31 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 102004039326	A1	20060216	DE 2004-102004039326	20040812
PRIORITY APPLN. INFO.:			DE 2004-102004039326	20040812

AB The invention discloses the use of one or more chemical or biol. substances to treat a neurodegenerative disease in a patient, whereby the chemical or biol. substance inhibits fatty acid amide hydrolase in all, essentially all, or specific cells of the patient and simultaneously not substantially cyclooxygenase-1 and/or cyclooxygenase-2 in all, essentially all, or specific body cells of the patient. The invention concerns further a procedure for the identification of the above chemical or biol. substances.
IT 681135-77-3, OL-135
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fatty acid amide hydrolase inhibitors for treatment of neurodegenerative disease, and screening method)
RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 17 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1216612 ZCAPLUS Full-text
DOCUMENT NUMBER: 144:100356
TITLE: Elucidation of Fatty Acid Amide Hydrolase Inhibition by Potent α-Ketoheterocycle Derivatives from Monte Carlo Simulations
AUTHOR(S): Guimaraes, Cristiano Ruch Werneck; Boger, Dale L.; Jorgensen, William L.
CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven,

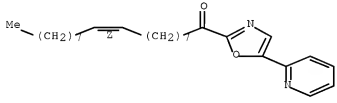
CT, 06520-8107, USA
SOURCE: Journal of the American Chemical Society (2005), 127(49), 17377-17384
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fatty acid amide hydrolase (FAAH) is a serine hydrolase responsible for the degradation of anandamide, an endogenous cannabinoid agonist, and oleamide, a sleep-inducing lipid. Recently, Boger and coworkers reported a potent, selective, and efficacious class of reversible α-ketoheterocycle inhibitors of FAAH that produce analgesia in animal models (J. Med. Chemical 2005, 48, 1849-1856; Bioorg. Med. Chemical Lett. 2005, 15, 1423-1428). Key aspects of the structure-activity data are addressed here through computational anal. of FAAH inhibition using Monte Carlo (MC) simulations in conjunction with free energy perturbation (FEP) calcns. The MC/FEP simulations demonstrate that incorporation of pyridine at the C5 position of the 2-keto-oxazole and 2-keto-1,3,4-oxadiazole derivs. significantly enhances binding affinity by formation of a hydrogen-bonded array between the pyridyl nitrogen and Lys142 and Thr236. The results also attribute the activity boost upon substitution of oxazole by oxadiazole to reduced steric interactions in the active site and a lower torsional energy penalty upon binding.

IT 639819-38-8 681135-40-0 808134-64-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(Monte Carlo simulations of fatty acid amide hydrolase inhibition by potent α-ketoheterocycle derivs.)

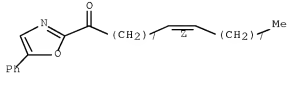
RN 639819-38-8 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



RN 681135-40-0 ZCAPLUS
CN 9-Octadecen-1-one, 1-(5-phenyl-2-oxazolyl)-, (9Z)- (CA INDEX NAME)

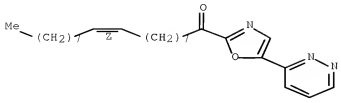
Double bond geometry as shown.



RN 808134-64-7 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(3-pyridazinyl)-2-oxazolyl]-, (9Z)- (CA INDEX

NAME)

Double bond geometry as shown.



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

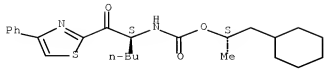
L31 ANSWER 18 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:708480 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:347441
TITLE: Ketoheterocycle-based inhibitors of cathepsin K: A novel entry into the synthesis of peptidic ketoheterocycles
AUTHOR(S): Tavares, Francis X.; Deaton, David N.; Miller, Aaron B.; Miller, Larry R.; Wright, Lois L.
CORPORATE SOURCE: Department of Medicinal Chemistry, GlaxoSmithKline, Research Triangle Park, NC, 27709, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(17), 3891-3895
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:347441

AB Ketoheterocyclic inhibitors of cathepsin K have been disclosed. SAR of potency enhancing P2-P3 groups coupled with ketoheterocyclic warheads to provide cathepsin K inhibitors have been described. In addition, a novel route to access α-ketothiazoles using a key thioamide functionality has been disclosed. The mild method employed allows for the presence of diverse functional groups, such as amide and carbamate functionalities, commonly found in protease inhibitors that have peptidomimetic scaffolds. This new method should provide a quick entry into functionally diverse protease inhibitors.

IT 865537-49-1P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation via key thioamide functionality and structure-activity relationship of ketoheterocycle-based inhibitors of cathepsin K)

RN 865537-49-1 ZCAPLUS
CN Carbamic acid, [(1S)-1-[(4-phenyl-2-thiazolyl)carbonyl]pentyl]-, (1S)-2-cyclohexyl-1-methylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



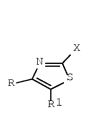
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 19 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:259684 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:336350
TITLE: Preparation of thiazole derivatives as cannabinoid receptor modulators
INVENTOR(S): Lange, Josephus H. M.; Kruse, Cornelis G.; Van Stuivenberg, Herman H.; Sliedregt, Leonardus A. J. M.
PATENT ASSIGNEE(S): Solvay Pharmaceuticals B.V., Neth.
SOURCE: U.S. Pat. Appl. Publ., 13 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

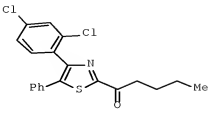
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050065189	A1	20050324	US 2004-942021	20040916
AU 2004274184	A1	20050331	AU 2004-274184	20040920
CA 2534798	A1	20050331	CA 2004-2534798	20040920
WO 2005028456	A1	20050331	WO 2004-EP52239	20040920
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1664005	A1	20060607	EP 2004-787171	20040920
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1849310	A	20061018	CN 2004-80024112	20040920
BR 2004014514	A	20061107	BR 2004-14514	20040920
JP 2007533621	T	20071122	JP 2006-526643	20040920
MX 2006PA02061	A	20060519	MX 2006-PA2061	20060222
IN 2006CN00941	A	20070615	IN 2006-CN941	20060317
NO 2006001701	A	20060616	NO 2006-1701	20060418

PRIORITY APPLN. INFO.:
EP 2003-78309 A 20030919
US 2003-504212P P 20030922
WO 2004-EP52239 W 20040920

OTHER SOURCE(S): CASREACT 142:336350; MARPAT 142:336350
GI



I



II

AB The present invention relates to a group of thiazole derivs. I [R, R1 = (un)substituted Ph, pyridyl; X = C(O)R2, C(O)NR3R4 (wherein R2 = alkyl, cycloalkyl, cycloalkylalkyl, etc.; R3 = H, alkyl; R4 = H, alkyl, cycloalkylalkyl, etc.; or NR3R4 = (un)saturated monocyclic or bicyclic heterocyclic group)], to methods for the preparation of these compds., to pharmaceutical compns. containing at least one compound I as active ingredient, as well to the use of these compns. for the treatment of psychiatric and neurol. disorders and other diseases involving cannabinoid CB neurotransmission. The thiazole derivs. I are either cannabinoid (CB) receptor antagonists, CB receptor agonists, CB receptor inverse agonists or CB receptor partial agonists. Twenty four compds. I were prepared E.g., a multi-step synthesis of II, starting from 1-(2,4-dichlorophenyl)-2-phenylethanone, was given. The compds. I were tested against human CB1 receptor and against human CB2 receptor binding (specific data were given for representative compds. I).

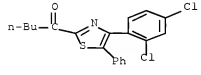
IT 848663-55-8P 848663-56-9P 848663-57-0P 848663-58-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of thiazole derivs. as cannabinoid receptor modulators for the treatment of psychiatric and neurol. disorders and other diseases involving cannabinoid CB neurotransmission)

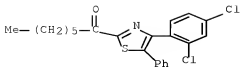
RN 848663-55-8 ZCAPLUS

CN 1-Pentanone, 1-[4-(2,4-dichlorophenyl)-5-phenyl-2-thiazolyl]- (CA INDEX NAME)

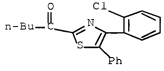


RN 848663-56-9 ZCAPLUS

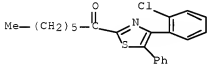
CN 1-Heptanone, 1-[4-(2,4-dichlorophenyl)-5-phenyl-2-thiazolyl]- (CA INDEX NAME)



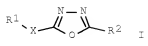
RN 848663-57-0 ZCAPLUS
CN 1-Pentanone, 1-[4-(2-chlorophenyl)-5-phenyl-2-thiazolyl]- (CA INDEX NAME)



RN 848663-58-1 ZCAPLUS
CN 1-Heptanone, 1-[4-(2-chlorophenyl)-5-phenyl-2-thiazolyl]- (CA INDEX NAME)



L31 ANSWER 20 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:130303 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:392343
TITLE: Discovery of an exceptionally potent and selective class of fatty acid amide hydrolase inhibitors enlisting proteome-wide selectivity screening: concurrent optimization of enzyme inhibitor potency and selectivity
AUTHOR(S): Leung, Donmienne; Du, Wu; Hardouin, Christophe; Cheng, Heng; Hwang, Inkyu; Cravatt, Benjamin F.; Boger, Dale L.
CORPORATE SOURCE: Department of Chemistry and the Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(5), 1423-1428
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:392343
GI



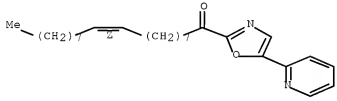
I

AB The concurrent implementation of a proteome-wide serine hydrolase selectivity screen with traditional efforts to optimize fatty acid amide hydrolase (FAAH) inhibition potency led to the expedited discovery of a new class of exceptionally potent (Ki < 300 pM) and unusually selective (>100-fold selective) inhibitors. These inhibitors are represented by disubstituted 1,3,4-oxadiazoles I [X = CH2, CO; R1 = (Z)- Me(CH2)7CH:CH(CH2)7, Ph(CH2)n; n = 5 - 8; R2 = Ph, 2-furyl, 2-pyridyl, 3-pyridyl, 4-pyridyl]. The iterative inhibitor design and evaluation with assistance of the selectivity screen served to differentiate otherwise indistinguishable inhibitors permitting the simultaneous optimization of potency and selectivity. Significantly, the simultaneous assessment of all potential competitive enzymes with the selectivity screen does not require the use of expressed or purified enzymes or a competitive substrate, no modification of the inhibitors is required, and the relative potency for competitive enzymes can be quantified (IC50's) including those that lack known substrates or function.

IT 639819-38-8 681135-40-0 681135-76-2
681135-77-3 681135-78-4 681135-79-5
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(optimization of potency and selectivity of fatty acid amide hydrolase inhibitors enlisting proteome-wide selectivity screening)

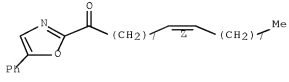
RN 639819-38-8 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

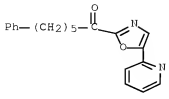


RN 681135-40-0 ZCAPLUS
CN 9-Octadecen-1-one, 1-(5-phenyl-2-oxazolyl)-, (9Z)- (CA INDEX NAME)

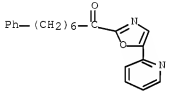
Double bond geometry as shown.



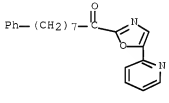
RN 681135-76-2 ZCAPLUS
CN 1-Hexanone, 6-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



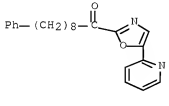
RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



RN 681135-78-4 ZCAPLUS
CN 1-Octanone, 8-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



RN 681135-79-5 ZCAPLUS
CN 1-Nonanone, 9-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

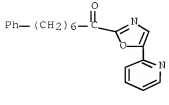


REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 21 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:906857 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:16687
TITLE: Reversible inhibitors of fatty acid amide hydrolase that promote analgesia: Evidence for an unprecedented combination of potency and selectivity
AUTHOR(S): Lichtman, Aron H.; Leung, Donmienne; Shelton, Christopher C.; Saghatelian, Alan; Hardouin, Christophe; Boger, Dale L.; Cravatt, Benjamin F.
CORPORATE SOURCE: Department of Pharmacology and Toxicology, School of Medicine, Virginia Commonwealth University, Richmond, VA, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (2004), 311(2), 441-448
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fatty acid amide hydrolase (FAAH) is the primary catabolic regulator of several bioactive lipid amides in vivo, including the endogenous cannabinoid anandamide and the sleep-inducing substance oleamide. Inhibitors of FAAH are considered a potential therapeutic approach for the treatment of several nervous system disorders, including pain, anxiety, and insomnia. However, for FAAH inhibitors to achieve clin. utility, they must not only display efficacy in vivo but also selectivity for this enzyme relative to the numerous other serine hydrolases present in mammalian proteomes. Here, we report a general strategy for evaluating the pharmacol. activity and target specificity of FAAH inhibitors and its implementation to develop the first class of selective reversible inhibitors of this enzyme that are highly efficacious in vivo. Using a series of functional proteomics, anal. chemical, and behavioral pharmacol. assays, we have identified a class of α-keto-heterocycles that show unprecedented selectivity for FAAH relative to other mammalian hydrolases, and, when administered to rodents, raise central nervous system levels of anandamide and promote cannabinoid receptor 1-dependent analgesia in several assays of pain sensation. These studies provide further evidence that FAAH may represent an attractive therapeutic target and describe a general route by which inhibitors of this enzyme can be optimized to achieve exceptional potency, selectivity, and efficacy in vivo.

IT 681135-77-3, OL 135
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(reversible inhibitors of fatty acid amide hydrolase that promote analgesia: evidence for an unprecedented combination of potency and selectivity)
RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

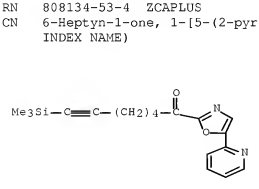


REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 22 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:890606 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:211392
TITLE: Discovery of a Potent, Selective, and Efficacious Class of Reversible α-Ketoheterocycle Inhibitors of Fatty Acid Amide Hydrolase Effective as Analgesics
AUTHOR(S): Boger, Dale L.; Miyauchi, Hiroshi; Du, Wu; Hardouin, Christophe; Fecik, Robert A.; Cheng, Heng; Hwang, Inkyu; Hedrick, Michael P.; Leung, Donmienne; Acevedo, Orlando; Guimaraes, Cristiano R. W.; Jorgensen, William L.; Cravatt, Benjamin F.
CORPORATE SOURCE: Departments of Chemistry Cell Biology and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of Medicinal Chemistry (2005), 48(6), 1849-1856
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:211392

AB Fatty acid amide hydrolase (FAAH) degrades neuromodulating fatty acid amides including anandamide (endogenous cannabinoid agonist) and oleamide (sleep-inducing lipid) at their sites of action and is intimately involved in their regulation. Herein the authors report the discovery of a potent, selective, and efficacious class of reversible FAAH inhibitors that produce analgesia in animal models validating a new therapeutic target for pain intervention. Key to the useful inhibitor discovery was the routine implementation of a proteomics-wide selectivity screen against the serine hydrolase superfamily ensuring selectivity for FAAH coupled with systematic in vivo examns. of candidate inhibitors.

IT 808134-53-4P
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(potent, selective, and efficacious reversible α-ketoheterocycle inhibitors of fatty acid amide hydrolase effective as analgesics)
RN 808134-53-4 ZCAPLUS
CN 6-Heptyn-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]-7-(trimethylsilyl)- (CA INDEX NAME)

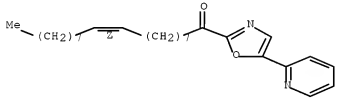


IT 639815-38-8P 681135-40-0P 681135-41-1P
681135-42-2P 681135-43-3P 681135-44-4P
681135-45-5P 681135-46-6P 681135-48-8P

681135-50-2P 681135-51-3P 681135-53-5P
681135-60-4P 681135-61-5P 681135-62-6P
681135-63-7P 681135-64-8P 681135-65-9P
681135-66-0P 681135-67-1P 681135-68-2P
681135-69-3P 681135-74-0P 681135-75-1P
681135-76-2P 681135-77-3P 681135-78-4P
681135-79-5P 681135-80-8P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-9-decene 681135-81-9P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-9-decyne 681135-82-0P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-9-octadecyne 681135-83-1P 681135-84-2P
681135-89-7P 808134-52-3P 808134-54-5P
808134-55-6P 808134-61-4P 808134-62-5P
808134-63-6P 808134-64-7P 808134-65-8P
808134-66-9P 808134-67-0P 808134-68-1P
808134-70-5P 808134-71-6P 808134-72-7P
808134-73-8P 808134-74-9P 808134-75-0P
808134-76-1P 808134-77-2P 808134-78-3P
808134-79-4P 808134-80-7P 808134-81-8P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(potent, selective, and efficacious reversible α-ketoheterocycle inhibitors of fatty acid amide hydrolase effective as analgesics)

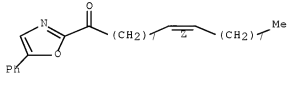
RN 639819-38-8 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



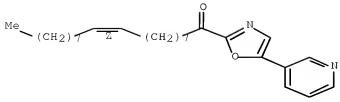
RN 681135-40-0 ZCAPLUS
CN 9-Octadecen-1-one, 1-(5-phenyl-2-oxazolyl)-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



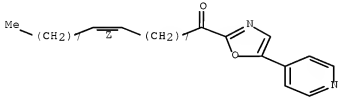
RN 681135-41-1 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(3-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



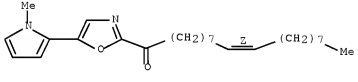
RN 681135-42-2 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(4-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



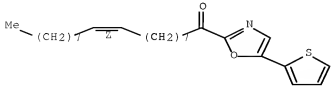
RN 681135-43-3 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(1-methyl-1H-pyrrol-2-yl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



RN 681135-44-4 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-thienyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

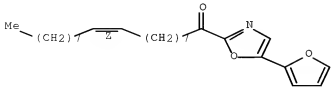
Double bond geometry as shown.



RN 681135-45-5 ZCAPLUS

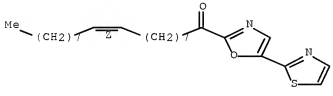
CN 9-Octadecen-1-one, 1-[5-(2-furanyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



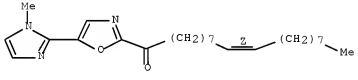
RN 681135-46-6 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-thiazolyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



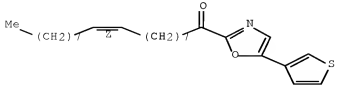
RN 681135-48-8 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(1-methyl-1H-imidazol-2-yl)-2-oxazolyl]-, (9Z)-
(CA INDEX NAME)

Double bond geometry as shown.



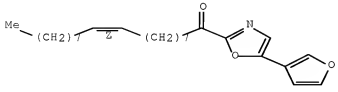
RN 681135-50-2 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(3-thienyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



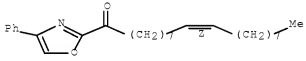
RN 681135-51-3 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(3-furanyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

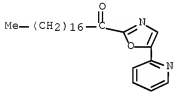


RN 681135-53-5 ZCAPLUS
CN 9-Octadecen-1-one, 1-(4-phenyl-2-oxazolyl)-, (9Z)- (CA INDEX NAME)

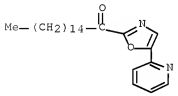
Double bond geometry as shown.



RN 681135-60-4 ZCAPLUS
CN 1-Octadecanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

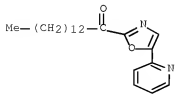


RN 681135-61-5 ZCAPLUS
CN 1-Hexadecanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

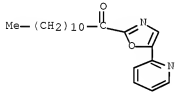


RN 681135-62-6 ZCAPLUS

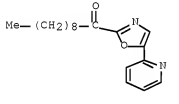
CN 1-Tetradecanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



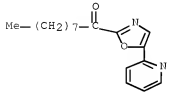
RN 681135-63-7 ZCAPLUS
CN 1-Dodecanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



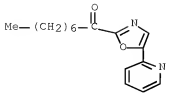
RN 681135-64-8 ZCAPLUS
CN 1-Decanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



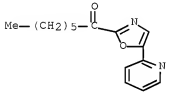
RN 681135-65-9 ZCAPLUS
CN 1-Nonanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



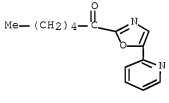
RN 681135-66-0 ZCAPLUS
CN 1-Octanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



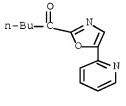
RN 681135-67-1 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



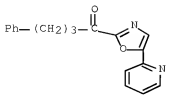
RN 681135-68-2 ZCAPLUS
CN 1-Hexanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



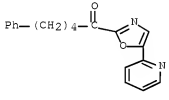
RN 681135-69-3 ZCAPLUS
CN 1-Pentanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



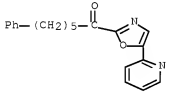
RN 681135-74-0 ZCAPLUS
CN 1-Butanone, 4-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



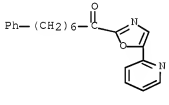
RN 681135-75-1 ZCAPLUS
CN 1-Pentanone, 5-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



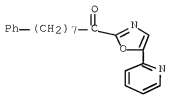
RN 681135-76-2 ZCAPLUS
CN 1-Hexanone, 6-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



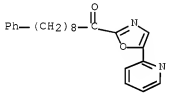
RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



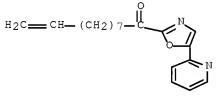
RN 681135-78-4 ZCAPLUS
CN 1-Octanone, 8-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



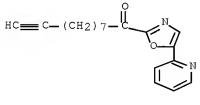
RN 681135-79-5 ZCAPLUS
CN 1-Nonanone, 9-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



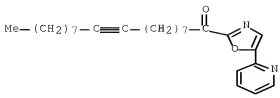
RN 681135-80-8 ZCAPLUS
CN 9-Decen-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



RN 681135-81-9 ZCAPLUS
CN 9-Decyn-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

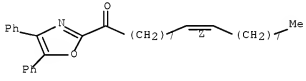


RN 681135-82-0 ZCAPLUS
CN 9-Octadecyn-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



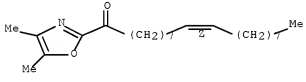
RN 681135-83-1 ZCAPLUS
CN 9-Octadecen-1-one, 1-(4,5-diphenyl-2-oxazolyl)-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

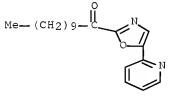


RN 681135-84-2 ZCAPLUS
CN 9-Octadecen-1-one, 1-(4,5-dimethyl-2-oxazolyl)-, (9Z)- (CA INDEX NAME)

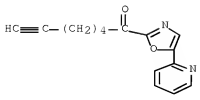
Double bond geometry as shown.



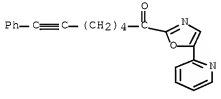
RN 681135-89-7 ZCAPLUS
CN 1-Undecanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



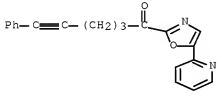
RN 808134-52-3 ZCAPLUS
CN 6-Heptyn-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



RN 808134-54-5 ZCAPLUS
CN 6-Heptyn-1-one, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

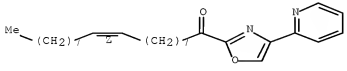


RN 808134-55-6 ZCAPLUS
CN 5-Hexyn-1-one, 6-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



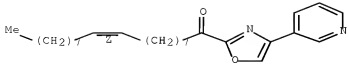
RN 808134-61-4 ZCAPLUS
CN 9-Octadecen-1-one, 1-[4-(2-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



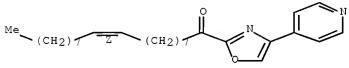
RN 808134-62-5 ZCAPLUS
CN 9-Octadecen-1-one, 1-[4-(3-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



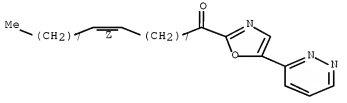
RN 808134-63-6 ZCAPLUS
CN 9-Octadecen-1-one, 1-[4-(4-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



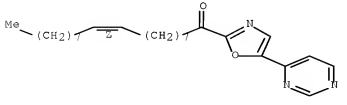
RN 808134-64-7 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(3-pyridazinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



RN 808134-65-8 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(4-pyrimidinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

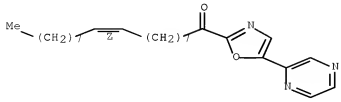
Double bond geometry as shown.



RN 808134-66-9 ZCAPLUS

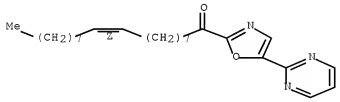
CN 9-Octadecen-1-one, 1-[5-(2-pyrazinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



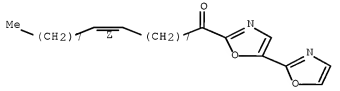
RN 808134-67-0 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-pyrimidinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

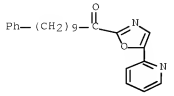


RN 808134-68-1 ZCAPLUS
CN 9-Octadecen-1-one, 1-[2,5'-bioxazol]-2'-yl-, (9Z)- (CA INDEX NAME)

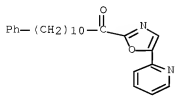
Double bond geometry as shown.



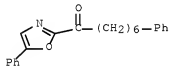
RN 808134-70-5 ZCAPLUS
CN 1-Decanone, 10-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



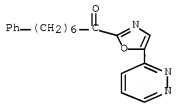
RN 808134-71-6 ZCAPLUS
CN 1-Undecanone, 11-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



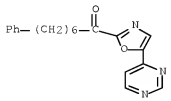
RN 808134-72-7 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-(5-phenyl-2-oxazolyl)- (CA INDEX NAME)



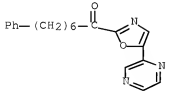
RN 808134-73-8 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(3-pyridazinyl)-2-oxazolyl]- (CA INDEX NAME)



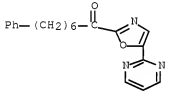
RN 808134-74-9 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(4-pyrimidinyl)-2-oxazolyl]- (CA INDEX NAME)



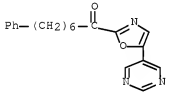
RN 808134-75-0 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyrazinyl)-2-oxazolyl]- (CA INDEX NAME)



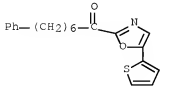
RN 808134-76-1 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyrimidinyl)-2-oxazolyl]- (CA INDEX NAME)



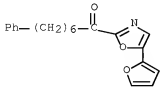
RN 808134-77-2 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(5-pyrimidinyl)-2-oxazolyl]- (CA INDEX NAME)



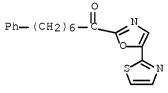
RN 808134-78-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-thienyl)-2-oxazolyl]- (CA INDEX NAME)



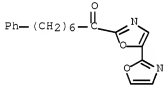
RN 808134-79-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-furanyl)-2-oxazolyl]-7-phenyl- (CA INDEX NAME)



RN 808134-80-7 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-thiazolyl)-2-oxazolyl]- (CA INDEX NAME)



RN 808134-81-8 ZCAPLUS
CN 1-Heptanone, 1-[2,5'-bioxazol]-2'-yl-7-phenyl- (CA INDEX NAME)



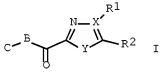
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 23 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:333840 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:339320
TITLE: Preparation of α-keto heterocycles as inhibitors of fatty acid amide hydrolase (FAAH)
INVENTOR(S): Boger, Dale L.
PATENT ASSIGNEE(S): The Scripps Research Institute, USA
SOURCE: PCT Int. Appl., 60 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

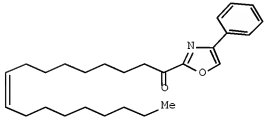
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004033652	A2	20040422	WO 2003-US31975	20031008
WO 2004033652	A3	20040916		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2501575	A1	20040422	CA 2003-2501575	20031008
AU 2003275493	A1	20040504	AU 2003-275493	20031008
EP 1549624	A2	20050706	EP 2003-759771	20031008
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003014980	A	20050809	BR 2003-14980	20031008
CN 1703407	A	20051130	CN 2003-80100994	20031008
JP 2006502229	T	20060119	JP 2004-543576	20031008
ZA 2005001837	A	20060628	ZA 2005-1837	20050303
MX 2005PA03762	A	20050722	MX 2005-PA3762	20050408
US 20060111359	A1	20060525	US 2005-528552	20050823
PRIORITY APPLN. INFO.:			US 2002-417247P P	20021008
			WO 2003-US31975 W	20031008

OTHER SOURCE(S): MARPAT 140:339320

GI



I



II

AB The invention is directed to the preparation of improved competitive inhibitors of fatty acid amide hydrolase FAAH (A–B–C), in particular I [A = α-keto heterocyclic inhibition subunit, i.e., oxazolyl, oxadiazolyl, thiazolyl; B = chain for linking the inhibition subunit A and the binding subunit C, i.e., linear skeleton of 3–9 atoms selected from C, O, S, N; C = binding subunit, i.e., π–bond containing radical, i.e., aryl, alkenyl, alkynyl, etc.;X = C, N; Y = O, S; R1, R2 = independently H, alkyl, hetero/aryl; provided that

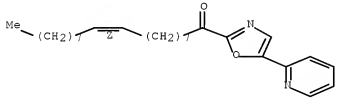
when R1 and R2 cannot both be H, and if X = N, R1 is absent]. The improved competitive inhibitors of FAAH display enhanced activity over conventional competitive inhibitors of FAAH. II was prepared by lithiation of 4-phenyloxazole with n-BuLi, transmetallated with ZnCl2, addition of CuI, and acylation of the in-situ formed cuprate with (Z)-9-octadecen-1-oyl chloride. The oxazoles and oxadiazoles are over 1,000 times more potent than the thiazoles. Selected I (10 mg/kg, i.p.) reduced thermal pain responses 60 min after administration in both the tail withdrawal test and hot plate test.

IT 639819-38-8P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-9-(Z)-octadecene
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(fatty acid amide hydrolase inhibitor; preparation of α-keto heterocycles as inhibitors of fatty acid amide hydrolase)

RN 639819-38-8 ZCAPLUS

CN 9-Octadecen-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

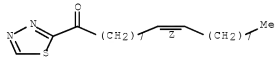


IT 681135-38-6P 681135-40-0P, 1-(5-Phenyloxazol-2-yl)-1-oxo-9-(Z)-octadecene 681135-41-1P, 1-Oxo-1-[5-(3-pyridyl)oxazol-2-yl]-9-(Z)-octadecene 681135-42-2P, 1-Oxo-1-[5-(4-pyridyl)oxazol-2-yl]-9-(Z)-octadecene 681135-43-3P, 1-[5-(1-Methylpyrrol-2-yl)oxazol-2-yl]-1-oxo-9-(Z)-octadecene 681135-44-4P, 1-Oxo-1-[5-(2-thienyl)oxazol-2-yl]-9-(Z)-octadecene 681135-45-5P, 1-[5-(2-Furyl)oxazol-2-yl]-1-oxo-9-(Z)-octadecene 681135-46-6P, 1-Oxo-1-[5-(thiazol-2-yl)oxazol-2-yl]-9-(Z)-octadecene 681135-48-8P, 1-Oxo-1-[5-(1-methylimidazol-2-yl)oxazol-2-yl]-9-(Z)-octadecene 681135-50-2P, 1-[5-(3-Thienyl)oxazol-2-yl]-1-oxo-9-(Z)-octadecene 681135-51-3P, 1-[5-(3-Furyl)oxazol-2-yl]-1-oxo-9-(Z)-octadecene 681135-53-5P, 1-(4-Phenyloxazol-2-yl)-1-oxo-9-(Z)-octadecene 681135-54-6P, 1-[4-(Pyridin-2-yl)oxazol-2-yl]octadec-9-en-1-one 681135-56-8P, 1-[4-(Pyridin-3-yl)oxazol-2-yl]octadec-9-en-1-one 681135-58-0P, 1-[4-(Pyridin-4-yl)oxazol-2-yl]octadec-9-en-1-one 681135-60-4P, 1-[5-(Pyridin-2-yl)oxazol-2-yl]octadecan-1-one 681135-61-5P, 1-[5-(Pyridin-2-yl)oxazol-2-yl]hexadecan-1-one 681135-62-6P, 1-[5-(Pyridin-2-yl)oxazol-2-yl]tetradecan-1-one 681135-63-7P, 1-[5-(Pyridin-2-yl)oxazol-2-yl]dodecan-1-one 681135-64-8P, 1-[5-(Pyridin-2-yl)oxazol-2-yl]decan-1-one 681135-65-9P, 1-[5-(Pyridin-2-yl)oxazol-2-yl]nonan-1-one 681135-66-0P, 1-[5-(Pyridin-2-yl)oxazol-2-yl]octan-1-one 681135-67-1P, 1-[5-(Pyridin-2-yl)oxazol-2-yl]heptan-1-one 681135-68-2P, 1-[5-(Pyridin-2-yl)oxazol-2-yl]hexan-1-one 681135-69-3P, 1-[5-(Pyridin-2-yl)oxazol-2-yl]pentan-1-one 681135-74-0P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-4-phenylbutane 681135-75-1P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-5-phenylpentane 681135-76-2P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-6-phenylhexane 681135-77-3P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-

7-phenylheptane 681135-78-4P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-8-phenyloctane 681135-79-5P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-9-phenylnonane 681135-80-8P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-9-decene 681135-81-9P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-9-decyne 681135-82-0P, 1-Oxo-1-[5-(2-pyridyl)oxazol-2-yl]-9-octadecyne 681135-83-1P, 1-(4,5-Diphenyloxazol-2-yl)-1-oxo-9-(Z)-octadecene 681135-84-2P, 1-(4,5-Dimethyloxazol-2-yl)-1-oxo-9-(Z)-octadecene
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(fatty acid amide hydrolase inhibitor; preparation of α-keto heterocycles as inhibitors of fatty acid amide hydrolase)

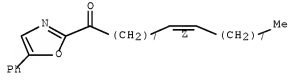
RN 681135-38-6 ZCAPLUS
CN 9-Octadecen-1-one, 1-(1,3,4-thiadiazol-2-yl)-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



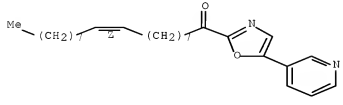
RN 681135-40-0 ZCAPLUS
CN 9-Octadecen-1-one, 1-(5-phenyl-2-oxazolyl)-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



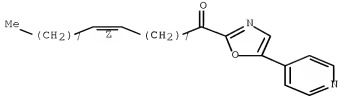
RN 681135-41-1 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(3-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



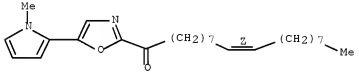
RN 681135-42-2 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(4-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



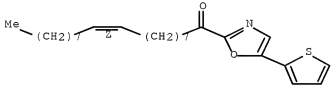
RN 681135-43-3 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(1-methyl-1H-pyrrol-2-yl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



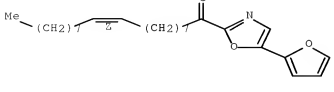
RN 681135-44-4 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-thienyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



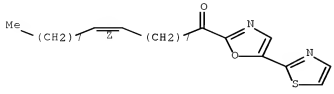
RN 681135-45-5 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-furanyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



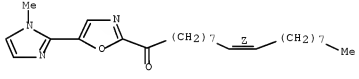
RN 681135-46-6 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-thiazolyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



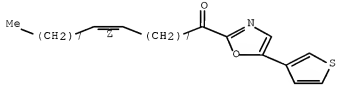
RN 681135-48-8 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(1-methyl-1H-imidazol-2-yl)-2-oxazolyl]-, (9Z)-
(CA INDEX NAME)

Double bond geometry as shown.



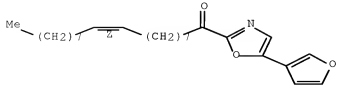
RN 681135-50-2 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(3-thienyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



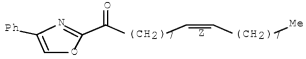
RN 681135-51-3 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(3-furanyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

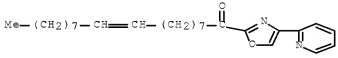


RN 681135-53-5 ZCAPLUS
CN 9-Octadecen-1-one, 1-(4-phenyl-2-oxazolyl)-, (9Z)- (CA INDEX NAME)

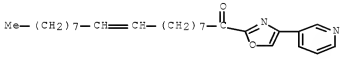
Double bond geometry as shown.



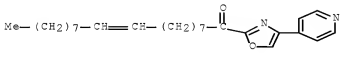
RN 681135-54-6 ZCAPLUS
CN 9-Octadecen-1-one, 1-[4-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



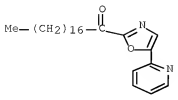
RN 681135-56-8 ZCAPLUS
CN 9-Octadecen-1-one, 1-[4-(3-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



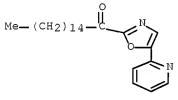
RN 681135-58-0 ZCAPLUS
CN 9-Octadecen-1-one, 1-[4-(4-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



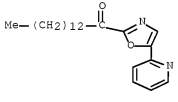
RN 681135-60-4 ZCAPLUS
CN 1-Octadecanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



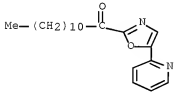
RN 681135-61-5 ZCAPLUS
CN 1-Hexadecanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



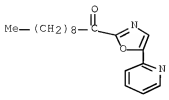
RN 681135-62-6 ZCAPLUS
CN 1-Tetradecanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



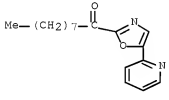
RN 681135-63-7 ZCAPLUS
CN 1-Dodecanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



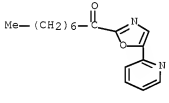
RN 681135-64-8 ZCAPLUS
CN 1-Decanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



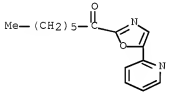
RN 681135-65-9 ZCAPLUS
CN 1-Nonanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



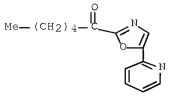
RN 681135-66-0 ZCAPLUS
CN 1-Octanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



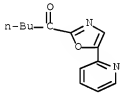
RN 681135-67-1 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



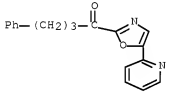
RN 681135-68-2 ZCAPLUS
CN 1-Hexanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



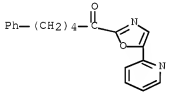
RN 681135-69-3 ZCAPLUS
CN 1-Pentanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



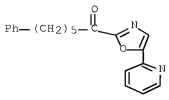
RN 681135-74-0 ZCAPLUS
CN 1-Butanone, 4-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



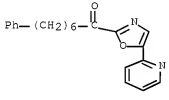
RN 681135-75-1 ZCAPLUS
CN 1-Pentanone, 5-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



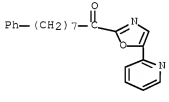
RN 681135-76-2 ZCAPLUS
CN 1-Hexanone, 6-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



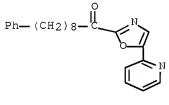
RN 681135-77-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



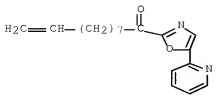
RN 681135-78-4 ZCAPLUS
CN 1-Octanone, 8-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



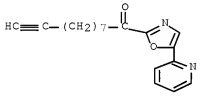
RN 681135-79-5 ZCAPLUS
CN 1-Nonanone, 9-phenyl-1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



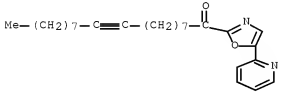
RN 681135-80-8 ZCAPLUS
CN 9-Decen-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



RN 681135-81-9 ZCAPLUS
CN 9-Decyn-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

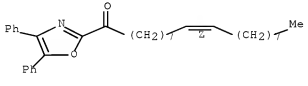


RN 681135-82-0 ZCAPLUS
CN 9-Octadecyn-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



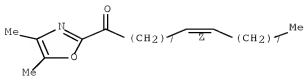
RN 681135-83-1 ZCAPLUS
CN 9-Octadecen-1-one, 1-(4,5-diphenyl-2-oxazolyl)-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

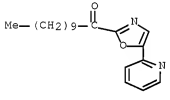


RN 681135-84-2 ZCAPLUS
CN 9-Octadecen-1-one, 1-(4,5-dimethyl-2-oxazolyl)-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.



IT 681135-89-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(fatty acid amide hydrolase inhibitor; preparation of α-keto heterocycles as inhibitors of fatty acid amide hydrolase)
RN 681135-89-7 ZCAPLUS
CN 1-Undecanone, 1-[5-(2-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)



L31 ANSWER 24 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:410694 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:72997
TITLE: Discovering potent and selective reversible inhibitors of enzymes in complex proteomes
AUTHOR(S): Leung, Donmienne; Hardouin, Christophe; Boger, Dale L.; Cravatt, Benjamin F.
CORPORATE SOURCE: The Skaggs Institute for Chemical Biology and the Department of Chemistry, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Nature Biotechnology (2003), 21(6), 687-691
CODEN: NABIF9; ISSN: 1087-0156
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English
AB To realize the promise of genomics-based therapeutics, new methods are needed to accelerate the discovery of small mols. that selectively modulate protein activity. Toward this end, advances in combinatorial synthesis have provided unprecedented access to large compound libraries of considerable structural complexity and diversity, shifting the bottleneck in drug discovery to the development of efficient screens for protein targets. Screening for reversible enzyme inhibitors typically requires extensive target-specific work, including protein expression and purification, as well as the development of specific substrate assays. Here we report a proteomic method for the discovery of reversible enzyme inhibitors that avoids these steps. We show that competitive profiling of a library of candidate serine hydrolase inhibitors in complex proteomes with activity-based chemical probes identifies nanomolar reversible inhibitors of several enzymes simultaneously, including the endocannabinoid-degrading enzyme fatty acid amide hydrolase (FAAH), triacylglycerol hydrolase (TGH) and an uncharacterized membrane-associated

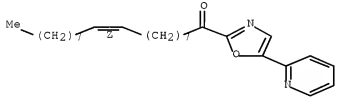
hydrolase that lacks known substrates. The strategy tests inhibitors against numerous enzymes in parallel, assigning both potency and selectivity factors to each agent. In this way, promiscuous inhibitors were readily rejected in favor of equally potent compds. with 500-fold or greater selectivity for their targets.

IT 639819-38-8
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(activity-based protein profiling of reversible inhibitors of enzymes in complex proteomes)

RN 639819-38-8 ZCAPLUS

CN 9-Octadecen-1-one, 1-[5-(2-pyridinyl)-2-oxazolyl]-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

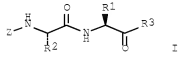


REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 25 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:	2002:640917 ZCAPLUS Full-text
DOCUMENT NUMBER:	138:56225
TITLE:	Solid-phase synthesis of peptidyl α-keto heterocycles
AUTHOR(S):	Subramanyam, Chakrapani; Chang, Shang Poa
CORPORATE SOURCE:	Groton Laboratories, Pfizer Global Research and Development, Groton, CT, 06340, USA
SOURCE:	Tetrahedron Letters (2002), 43(36), 6313-6315 CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER:	Elsevier Science Ltd.
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 138:56225

GI



I

AB The synthesis of structurally diverse peptidyl α-keto heterocycles I [R1 = CH2Ph, R2 = CH2Ph, R3 = Ph; R1 = CH2CH2Ph, R2 = CH2Ph, R3 = 2-furyl, 2-thiophenyl, 2-thiazolyl, 2- benzothiazolyl, 2-benzoxazolyl, 2-(4-phenyl)-oxazolyl, 2-oxazolyl, or 4-oxazolyl; Z = benzyloxycarbonyl] via solid-phase

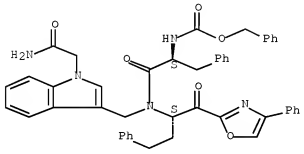
method from corresponding amino acid allyl esters and hetero arenes is reported.

IT 479421-10-8DP, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase synthesis of peptidyl keto heterocycles from corresponding amino acid allyl esters and hetero arenes)

RN 479421-10-8 ZCAPLUS

CN Carbamic acid, [(1S)-2-[[[1-(2-amino-2-oxoethyl)-1H-indol-3-yl]methyl][(1S)-3-phenyl-1-[(4-phenyl-2-oxazolyl)carbonyl]propyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

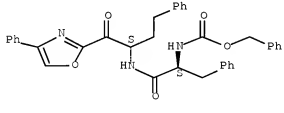


IT 479420-93-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of peptidyl keto heterocycles from corresponding amino acid allyl esters and hetero arenes)

RN 479420-93-4 ZCAPLUS

CN Carbamic acid, [(1S)-2-oxo-1-(phenylmethyl)-2-[[(1S)-3-phenyl-1-[(4-phenyl-2-oxazolyl)carbonyl]propyl]amino]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 26 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:412634 ZCAPLUS Full-text
DOCUMENT NUMBER: 135:162089
TITLE: 4-Hydroxy-5,6-dihydropyrones as inhibitors of HIV protease: the effect of heterocyclic substituents at C-6 on antiviral potency and pharmacokinetic

parameters

AUTHOR(S): Hagen, Susan E.; Domagala, John; Gajda, Christopher; Lovdahl, Michael; Tait, Bradley D.; Wise, Eric; Holler, Tod; Hupe, Donald; Nouhan, Carolyn; Urumov, Andrej; Zeikus, Greg; Zeikus, Eric; Lunney, Elizabeth A.; Pavlovsky, Alexander; Gracheck, Stephen J.; Saunders, James; VanderRoest, Steve; Brodfuehrer, Joanne

CORPORATE SOURCE: Departments of Chemistry Biochemistry Biomolecular Structure and Drug Design Infectious Diseases, Pfizer Global Research and Development, Ann Arbor, MI, 48105, USA

SOURCE: Journal of Medicinal Chemistry (2001), 44(14), 2319-2332
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

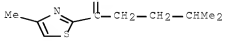
OTHER SOURCE(S): CASREACT 135:162089

AB Due largely to the emergence of multi-drug-resistant HIV strains, the development of new HIV protease inhibitors remains a high priority for the pharmaceutical industry. Toward this end, the authors previously identified a 4-hydroxy-5,6-dihydropyrone lead compound (CI-1029) which possesses excellent activity against the protease enzyme, good antiviral efficacy in cellular assays, and promising bioavailability in several animal species. The search for a suitable back-up candidate centered on the replacement of the aniline moiety at C-6 with an appropriately substituted heterocycle. In general, this series of heterocyclic inhibitors displayed good activity (in both enzymic and cellular tests) and low cellular toxicity; furthermore, several analogs exhibited improved pharmacokinetic parameters in animal models. The compound with the best combination of high potency, low toxicity, and favorable bioavailability was (S)-3-(2-tert-butyl-4-hydroxymethyl-5-methyl-phenylsulfanyl)-4-hydroxy- 6-isopropyl-6-(2-thiophen-3-yl-ethyl)-5,6-dihydro-pyran-2-one (I). This thiophene derivative also exhibited excellent antiviral efficacy against mutant HIV protease and resistant HIV strains. For these reasons, I was chosen for further preclin. evaluation.

IT 354581-35-4P 354581-36-5P 354581-40-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hydroxydihydropyrones as inhibitors of HIV protease and effect of heterocyclic substituents at C-6 on antiviral potency and pharmacokinetic parameters and toxicity in relation to drug resistance)

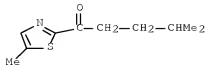
RN 354581-35-4 ZCAPLUS

CN 1-Pentanone, 4-methyl-1-(4-methyl-2-thiazolyl)- (CA INDEX NAME)

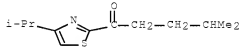


RN 354581-36-5 ZCAPLUS

CN 1-Pentanone, 4-methyl-1-(5-methyl-2-thiazolyl)- (CA INDEX NAME)



RN 354581-40-1 ZCAPLUS
CN 1-Pentanone, 4-methyl-1-[4-(1-methylethyl)-2-thiazolyl]- (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 27 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:78357 ZCAPLUS Full-text
DOCUMENT NUMBER: 134:131708
TITLE: Preparation and bioactivity of vitamin D derivs. with cyclic substructures in the side chains
INVENTOR(S): Steinmeyer, Andreas; Schwarz, Katica; Giesen, Claudia; Haberey, Martin; Fahnrich, Marianne
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 134 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007405	A2	20010201	WO 2000-EP7104	20000724
WO 2001007405	A3	20020328		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19935771	A1	20010201	DE 1999-19935771	19990723
CA 2376465	A1	20010201	CA 2000-2376465	20000724
BR 2000013175	A	20020402	BR 2000-13175	20000724
EP 1210327	A2	20020605	EP 2000-962278	20000724
EP 1210327	B1	20060118		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
HU 2002002015	A2	20021028	HU 2002-2015	20000724

HU 2002002015	A3	20040428			
JP 2003505447	T	20030212	JP 2001-512492		20000724
EE 200200036	A	20030415	EE 2002-36		20000724
EE 5027	B1	20080616			
US 6603031	B1	20030805	US 2000-624608		20000724
EP 1362848	A1	20031119	EP 2003-90212		20000724
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY					
NZ 515891	A	20040326	NZ 2000-515891		20000724
AU 773673	B2	20040603	AU 2000-74072		20000724
AT 316073	T	20060215	AT 2000-962278		20000724
ES 2254222	T3	20060616	ES 2000-962278		20000724
EE 200800025	A	20080616	EE 2008-25		20000724
IN 2001MN01587	A	20060106	IN 2001-MN1587		20011213
MX 2001PA13330	A	20020709	MX 2001-PA13330		20011219
BG 106334	A	20020628	BG 2002-106334		20020121
NO 2002000330	A	20020322	NO 2002-330		20020122
ZA 2002001482	A	20030521	ZA 2002-1482		20020221
US 20030149006	A1	20030807	US 2002-303916		20021126
US 7115758	B2	20061003			
IN 2005MN01178	A	20070706	IN 2005-MN1178		20051025
IN 2005MN01185	A	20070817	IN 2005-MN1185		20051025
PRIORITY APPLN. INFO.:			DE 1999-19935771	A	19990723
			EE 2002-36	A	20000724
			EP 2000-962278	A3	20000724
			US 2000-624608	A3	20000724
			WO 2000-EP7104	W	20000724
			IN 2001-MN1587	A3	20011213

OTHER SOURCE(S): MARPAT 134:131708
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

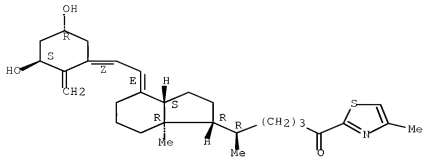
AB The invention describes the synthesis of vitamin D derivs. [I; Y1, Y2 = OH, alkanoyloxy, aroyloxy; R1, R2 = H; R1R2 = CH2; R3, R4 = H, Cl, F, alkyl, etc.; Q = alkylene chain; X1, X2 = H, OH, Cl, F, Br, etc.; Z = (un)substituted, (un)saturated or aromatic 5-, 6-membered carbo-, heterocyclic ring], the intermediates used in the process, and the production of medicaments. Thus, vitamin D analog II was prepared via Wittig reaction of ketone III (also prepared) with IV, followed by deprotection. II had competition factor of 5 vs. calcitriol towards receptor binding and dose relation for differentiation induction in HL 60 cell.

IT 321909-60-8P 321911-26-6P 321912-03-2P
321912-06-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and bioactivity of vitamin D derivs. with cyclic substructures in the side chains)

RN 321909-60-8 ZCAPLUS

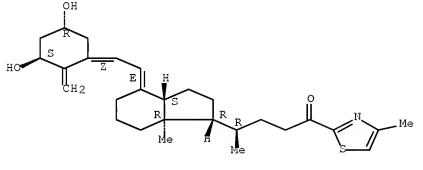
CN 1-Hexanone, 5-[(1R,3aS,4E,7aR)-4-[(2Z)-2-[(3S,5R)-3,5-dihydroxy-2-methylenecyclohexylidene]ethylidene]octahydro-7a-methyl-1H-inden-1-yl]-1-(4-methyl-2-thiazolyl)-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



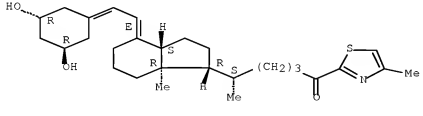
RN 321911-26-6 ZCAPLUS
CN 1-Pentanone, 4-[(1R,3aS,4E,7aR)-4-[(2Z)-2-[(3S,5R)-3,5-dihydroxy-2-methylenecyclohexylidene]ethylidene]octahydro-7a-methyl-1H-inden-1-yl]-1-(4-methyl-2-thiazolyl)-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 321912-03-2 ZCAPLUS
CN 1-Hexanone, 5-[(1R,3aS,4E,7aR)-4-[2-[(3R,5R)-3,5-dihydroxycyclohexylidene]ethylidene]octahydro-7a-methyl-1H-inden-1-yl]-1-(4-methyl-2-thiazolyl)-, (5S)- (CA INDEX NAME)

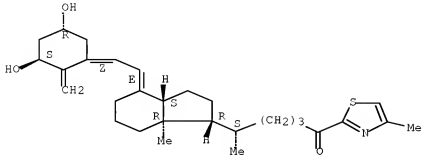
Absolute stereochemistry.
Double bond geometry as shown.



RN 321912-06-5 ZCAPLUS
CN 1-Hexanone, 5-[(1R,3aS,4E,7aR)-4-[(2Z)-2-[(3S,5R)-3,5-dihydroxy-2-methylenecyclohexylidene]ethylidene]octahydro-7a-methyl-1H-inden-1-yl]-1-

(4-methyl-2-thiazolyl)-, (5S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

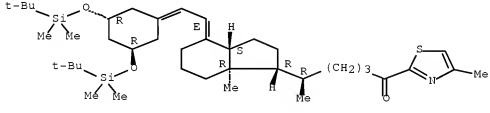


IT 321909-54-0P 321909-59-5P 321911-25-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bioactivity of vitamin D derivs. with cyclic substructures in the side chains)

RN 321909-54-0 ZCAPLUS

CN 1-Hexanone, 5-[(1R,3aS,4E,7aR)-4-[2-[(3R,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]cyclohexylidene]ethylidene]octahydro-7a-methyl-1H-inden-1-yl]-1-(4-methyl-2-thiazolyl)-, (5R)- (CA INDEX NAME)

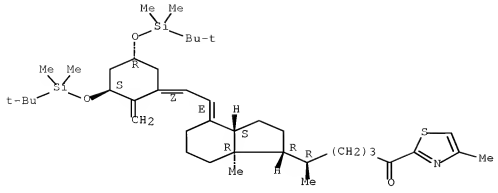
Absolute stereochemistry.
Double bond geometry as shown.



RN 321909-59-5 ZCAPLUS

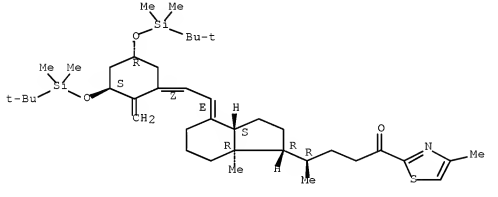
CN 1-Hexanone, 5-[(1R,3aS,4E,7aR)-4-[(2Z)-2-[(3S,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methylenecyclohexylidene]ethylidene]octahydro-7a-methyl-1H-inden-1-yl]-1-(4-methyl-2-thiazolyl)-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



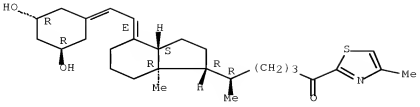
RN 321911-25-5 ZCAPLUS
CN 1-Pentanone, 4-[(1R,3aS,4E,7aR)-4-[(2Z)-2-[(3S,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-methylenecyclohexylidene]ethylidene]octahydro-7a-methyl-1H-inden-1-yl]-1-(4-methyl-2-thiazolyl)-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 321909-55-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and bioactivity of vitamin D derivs. with cyclic substructures in the side chains)
RN 321909-55-1 ZCAPLUS
CN 1-Hexanone, 5-[(1R,3aS,4E,7aR)-4-[2-[(3R,5R)-3,5-dihydroxycyclohexylidene]ethylidene]octahydro-7a-methyl-1H-inden-1-yl]-1-(4-methyl-2-thiazolyl)-, (5R)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



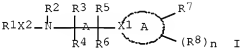
L31 ANSWER 28 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:666718 ZCAPLUS Full-text
DOCUMENT NUMBER: 133:252041
TITLE: Preparation of amine derivatives as cathepsin K and cathepsin S inhibitors and in treating pathology and/or symptomatology of diseases caused by cysteine protease activity
INVENTOR(S): Link, John O.; Martelli, Arnold J.; Martichonok, Valeri; Patterson, John W.; Saunders, Oliver L.; Zipfel, Sheila
PATENT ASSIGNEE(S): Axys Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 223 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000055144	A1	20000921	WO 2000-US6885	20000315
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2367352	A1	20000921	CA 2000-2367352	20000315
AU 2000037507	A	20001004	AU 2000-37507	20000315
AU 774664	B2	20040701		
EP 1161422	A1	20011212	EP 2000-916397	20000315
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000009044	A	20020115	BR 2000-9044	20000315
TR 200103335	T2	20020422	TR 2001-3335	20000315
HU 2002000572	A2	20020629	HU 2002-572	20000315
HU 2002000572	A3	20040728		
JP 2002539201	T	20021119	JP 2000-605574	20000315
EE 200100486	A	20030217	EE 2001-486	20000315
US 6576630	B1	20030610	US 2000-525507	20000315
EP 1516877	A1	20050323	EP 2004-15656	20000315
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
ZA 2001007496	A	20021211	ZA 2001-7496	20010911
MX 2001PA09240	A	20020108	MX 2001-PA9240	20010913

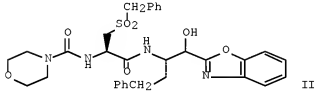
IN 2001KN00948	A	20050311	IN 2001-KN948		20010913
NO 2001004483	A	20011101	NO 2001-4483		20010914
BG 105969	A	20020531	BG 2001-105969		20011002
HR 2001000736	A1	20021231	HR 2001-736		20011012
US 20030232864	A1	20031218	US 2003-354888		20030128
AU 2004201071	A1	20040408	AU 2004-201071		20040315
PRIORITY APPLN. INFO.:			US 1999-124421P	P	19990315
			AU 2000-37507	A3	20000315
			EP 2000-916397	A3	20000315
			US 2000-525507	A1	20000315
			WO 2000-US6885	W	20000315

OTHER SOURCE(S): MARPAT 133:252041

GI



I



II

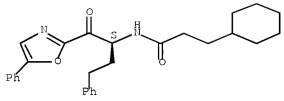
AB Title compds. [I; A = heteromonocyclic ring containing 5-6 member; fused heteropolycyclic ring containing 8-14 member; X1 = C, CH; X2 = bond, NHCH2CO, NHCH2CH2SO2, alkylamino; R1 = alkylaminocarbonyl, alkoxycarbonyl, alkylcarbonyl, alkylsulfonyl; R2 = H, alkyl; R3 = alkyl; R4 = H, alkyl; R3R4 = cycloalkylene, heterocycloalkylene; R5 = H; R6 = H; R5R6 = oxo; R7 = CN, Cl, Br, F, NO2, H; R8 = alkyl, alkylidene, CN, Cl, F, Br, NO2; n = 0, 1, 2, 3], N-oxide derivs., prodrug derivs., protected derivs., individual isomers, mixts. of isomers, and pharmaceutically acceptable salts and compns. with bisphosphonic acids or acid esters as excipients are prepared as cathepsin K and cathepsin S inhibitors. Title compds. are administering to animal in treating diseases which cysteine protease activity contributes to the pathol. and/or symptomatol. The diseases are autoimmune disorder, allergic disorder, allogeneic immune response, excessive elastolysis, cardiovascular disorders, fibril formation, etc. Thus, the title compound II was prepared

IT 294882-87-4P 294882-88-5P 294885-02-2P
294885-03-3P 294885-04-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amine derivs. as cathepsin K and cathepsin S inhibitors useful in disorders caused by cysteine protease activity)

RN 294882-87-4 ZCAPLUS

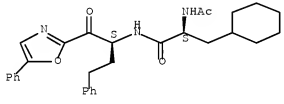
CN Cyclohexanepropanamide, N-[(1S)-3-phenyl-1-[(5-phenyl-2-oxazolyl)carbonyl]propyl]- (CA INDEX NAME)

Absolute stereochemistry.



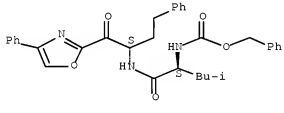
RN 294882-88-5 ZCAPLUS
CN Cyclohexanepropanamide, α-(acetylamino)-N-[(1S)-3-phenyl-1-[(5-phenyl-2-oxazolyl)carbonyl]propyl]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



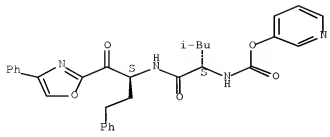
RN 294885-02-2 ZCAPLUS
CN Carbamic acid, [(1S)-3-methyl-1-[[[(1S)-3-phenyl-1-[(4-phenyl-2-oxazolyl)carbonyl]propyl]amino]carbonyl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



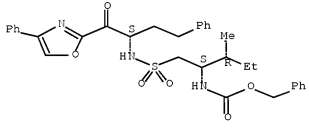
RN 294885-03-3 ZCAPLUS
CN Carbamic acid, [(1S)-3-methyl-1-[[[(1S)-3-phenyl-1-[(4-phenyl-2-oxazolyl)carbonyl]propyl]amino]carbonyl]butyl]-, 3-pyridinyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 294885-04-4 ZCAPLUS
CN Carbamic acid, [(1S,2R)-2-methyl-1-[[[[(1S)-3-phenyl-1-[(4-phenyl-2-oxazolyl)carbonyl]propyl]amino]sulfonyl]methyl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 29 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:628128 ZCAPLUS Full-text
DOCUMENT NUMBER: 133:208196
TITLE: Preparation of peptides as reversible inhibitors of cathepsin S
INVENTOR(S): Cywin, Charles L.; Frye, Leah L.; Morwick, Tina; Spero, Denice M.; Thomson, David; Ward, Yancey
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 315 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000051998	A1	20000908	WO 1999-US26278	19991105
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2360740	A1	20000908	CA 1999-2360740	19991105
EP 1159273	A1	20011205	EP 1999-973745	19991105
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, FI

US 6395897	B1	20020528	US 1999-434106	19991105
JP 2002538151	T	20021112	JP 2000-602225	19991105
MX 2001PA08713	A	20020225	MX 2001-PA8713	20010828
US 20020091259	A1	20020711	US 2001-82952	20011024
US 6608057	B2	20030819		
US 20030158406	A1	20030821	US 2003-366282	20030213
US 6730671	B2	20040504		

PRIORITY APPLN. INFO.:

US 1999-122570P	P	19990302
US 1999-434106	A1	19991105
WO 1999-US26278	W	19991105
US 2001-82952	A3	20011024

OTHER SOURCE(S): MARPAT 133:208196

AB Compds. R1-A-NHCR2R3C(:X)NR4CR5R6R7 [A = C:O, C:S, C:NH or substituted imino group; R1 = (un)substituted alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl, amino; R2, R4 = H, alkyl; R3, R6 = H or (un)substituted alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl; R5 = H, alkyl, cycloalkyl; R7 = R8C(Z), where Z = O, S, NH or substituted derivative and R8 is (un)substituted 5-8 membered monocyclic or 8-11 membered bicyclic heteroaryl having 1-4 heteroatoms selected from N, O and S; X = O, S, NOH] were prepared as cathepsin S inhibitors. Thus, morpholine-4-carboxylic acid [1-(S)-[1-(S)-cyano-3-phenylpropylcarbamoyl]-3-methylbutyl]amide was prepared by coupling L-homophenylalaninamide with N-(4-morpholinecarbonyl)-L- leucine and reaction with cyanuric chloride. Compds. of the invention were evaluated for inhibition of cathepsin S (IC50 ≤ 100 μM).

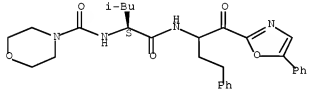
IT 290817-04-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptides as reversible inhibitors of cathepsin S)

RN 290817-04-8 ZCAPLUS

CN 4-Morpholinecarboxamide, N-[(1S)-3-methyl-1-[[[3-phenyl-1-[(5-phenyl-2-oxazolyl)carbonyl]propyl]amino]carbonyl]butyl]- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 30 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:275284 ZCAPLUS Full-text

DOCUMENT NUMBER: 131:53581

TITLE: Potent and selective bicyclic lactam inhibitors of thrombin: Part 3: P1' modifications

AUTHOR(S): Plummer, Janet S.; Berryman, Kent A.; Cai, Cuiman; Cody, Wayne L.; DiMaio, John; Doherty, Annette M.; Eaton, Scott; Edmunds, Jeremy J.; Holland, Debra R.; Lafleur, D.; Levesque, Sophie; Narasimhan, Lakshmi S.; Rubin, J. Ronald; Rapundalo, Stephen T.; Siddiqui, M.

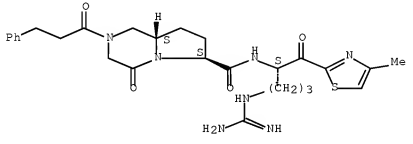
Arshad; Susser, A.; St. Denis, Yves; Winocour, Peter
CORPORATE SOURCE: Parke-Davis Pharmaceutical Research, Division of Warner-Lambert Company, Ann Arbor, MI, 48105, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(6), 835-840
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis and antithrombotic activity of a series of nonpeptide bicyclic thrombin inhibitors are described. We have explored the SAR around the P1' site. Modification of the P1' site has been found to affect potency and selectivity.

IT 227962-87-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bicyclic lactam inhibitors of thrombin)

RN 227962-87-0 ZCAPLUS
CN Pyrrolo[1,2-a]pyrazine-6-carboxamide, N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(4-methyl-2-thiazolyl)carbonyl]butyl]octahydro-4-oxo-2-(1-oxo-3-phenylpropyl)-, (6S,8aS)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 31 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:12363 ZCAPLUS Full-text
DOCUMENT NUMBER: 130:52744
TITLE: Preparation of thrombin inhibitors containing a peptidyl heterocycle
INVENTOR(S): De Man, A. P. A.; Peters, J. A. M.; Van Aelst, S. F.; Adang, A. E. P.
PATENT ASSIGNEE(S): Akzo Nobel N.V., Neth.
SOURCE: Eur. Pat. Appl., 8 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 884325	A1	19981216	EP 1998-201280	19980421

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

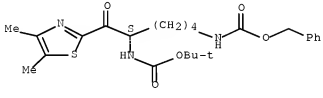
US 5877156 A 19990302 US 1998-63484 19980421
PRIORITY APPLN. INFO.: EP 1997-201217 A 19970424
OTHER SOURCE(S): MARPAT 130:52744

AB Thrombin inhibitors R1NHCHR2CO-A-B-X [R1 is alkylene-CO2H or -CONH2; R2 is a side chain of a hydrophobic D-amino acid; A is an amino acid selected from proline, optionally containing a second heteroatom selected from N, O, or S, and optionally substituted with alkyl, alkoxy or halogen, 2-azetidinecarboxylic acid, pipecolinic acid, octahydroindole-2-carboxylic acid or valine; B is lysine, 3- or 4-aminocyclohexylglycine or ω-alkyl-lysine; and X is (un)substituted 2-thiazolyl, 2-thiazolinyl, 2-benzothiazolyl, 2-oxazolyl, 2-oxazolinyl, 2-benzoxazolyl, 2-imidazolyl, or 2-benzimidazolyl] or their pharmaceutically acceptable salts were prepared Thus, 2-(N-carboxymethyl-D-cyclohexylalanylprolyllysinyl)-4,5- dimethylthiazole was prepared via peptide coupling in solution of N-(Boc-methyl)-N-Boc-D-Cha-OH (Boc = tert-butoxycarbonyl, Cha = cyclohexylalaninyl), H-Pro-OBzl.HCl, and 2-(N-benzyloxycarbonyl)lysinyl- 4,5-dimethylthiazole.

IT 217457-44-8P 217457-45-9P 217457-46-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of thrombin inhibitors containing peptidyl heterocycle)

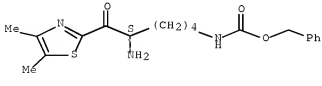
RN 217457-44-8 ZCAPLUS
CN Carbamic acid, [(5S)-5-[[(1,1-dimethylethoxy)carbonyl]amino]-6-(4,5-dimethyl-2-thiazolyl)-6-oxohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



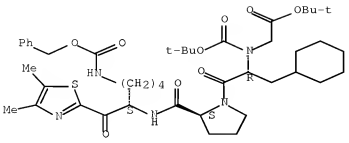
RN 217457-45-9 ZCAPLUS
CN Carbamic acid, [(5S)-5-amino-6-(4,5-dimethyl-2-thiazolyl)-6-oxohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



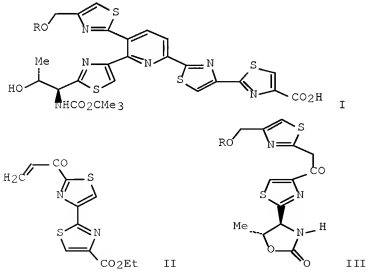
RN 217457-46-0 ZCAPLUS
CN L-Prolinamide, 3-cyclohexyl-N-[(1,1-dimethylethoxy)carbonyl]-N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-D-alanyl-N-[(1S)-1-[(4,5-dimethyl-2-thiazolyl)carbonyl]-5-[[(phenylmethoxy)carbonyl]amino]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 32 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:339409 ZCAPLUS Full-text
DOCUMENT NUMBER: 127:50975
ORIGINAL REFERENCE NO.: 127:9733a,9736a
TITLE: Studies toward Thiostrepton Antibiotics: Assembly of the Central Pyridine-Thiazole Cluster of Micrococcins
AUTHOR(S): Ciufolini, Marco A.; Shen, Yong Chun
CORPORATE SOURCE: Department of Chemistry, Rice University, Houston, TX, 77005-1892, USA
SOURCE: Journal of Organic Chemistry (1997), 62(12), 3804-3805
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:50975
GI



I

II III

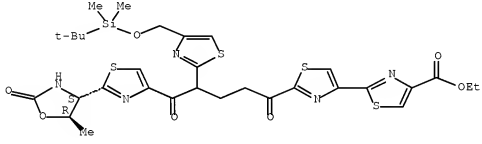
AB A convergent synthesis of acid I (R = SiMe2CMe3), which contains the pyridine-thiazole skeleton of micrococcin P1, was described. Key to the synthesis was the Michael addition of propenoyl substituted bithiazole II with bis-thiazolylethanone III (R = SiMe2CMe3) in nearly quant. yield.

IT 190523-45-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of the central pyridine-thiazole cluster of the thiostrepton antibiotic, micrococcin P1)

RN 190523-45-6 ZCAPLUS

CN [2,4'-Bithiazole]-4-carboxylic acid, 2'-[4-[4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-thiazolyl]-5-[2-[(4S,5R)-5-methyl-2-oxo-4-oxazolidinyl]-4-thiazolyl]-1,5-dioxopentyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 33 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN

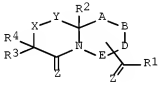
ACCESSION NUMBER:	1996:509465 ZCAPLUS Full-text
DOCUMENT NUMBER:	125:167970
ORIGINAL REFERENCE NO.:	125:31480h,31481a
TITLE:	Low molecular weight bicyclic thrombin inhibitors
INVENTOR(S):	Dimaio, John; Siddiqui, M. Arshad; Gillard, John W.; St-Denis, Yves; Tarazi, Micheline; Preville, Patrice; Levesque, Sophie; Bachand, Benoit
PATENT ASSIGNEE(S):	Biochem Pharma Inc., Can.
SOURCE:	PCT Int. Appl., 182 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9619483	A1	19960627	WO 1995-CA708	19951221
W: AL, AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,				

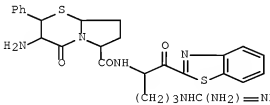
SI, SK
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

CA 2208772	A1	19960627	CA 1995-2208772		19951221
AU 9642505	A	19960710	AU 1996-42505		19951221
EP 802916	A1	19971029	EP 1995-940923		19951221
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV					
CN 1175259	A	19980304	CN 1995-197614		19951221
HU 77651	A2	19980728	HU 1998-216		19951221
BR 9510433	A	19981110	BR 1995-10433		19951221
NZ 297360	A	20000327	NZ 1995-297360		19951221
AU 9540628	A	19960704	AU 1995-40628		19951222
AU 715378	B2	20000203			
ZA 9510960	A	19960709	ZA 1995-10960		19951222
ZA 9510961	A	19960709	ZA 1995-10961		19951222
FI 9702466	A	19970819	FI 1997-2466		19970611
NO 9702892	A	19970820	NO 1997-2892		19970620
US 6057314	A	20000502	US 1997-880885		19970623
LV 12019	B	19980720	LV 1997-141		19970715
LT 4368	B	19980825	LT 1997-132		19970721
PRIORITY APPLN. INFO.:			GB 1994-26038	A	19941222
			GB 1995-3136	A	19950217
			GB 1995-10265	A	19950522
			GB 1995-10266	A	19950522
			GB 1995-10267	A	19950522
			WO 1995-CA708	W	19951221

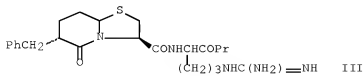
OTHER SOURCE(S): MARPAT 125:167970
GI



I



II



III

AB Heterobicyclic thrombin inhibitors I (A, B = CH, S, O, etc.; D = CH, C-alkyl, etc.; E = CH2, CH-acyl; X = O, NH, etc.; Y = O, S, SO, etc.; Z = O, S, etc.;

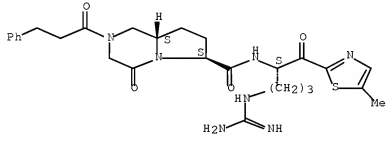
R1 = e.g., arginyl moiety substituted with an amino acid or heterocycle; R2 = H or organyl; R3 = H, amino, etc.; R4 = H, aryl, cycloalkyl, etc.) were prepared Thus, benzothiazole derivative II was prepared in 7 steps from PhCH2SCH2CH(NHCBz)COOH and 4-hydroxyproline. In a fibrin clotting assay with human thrombin and bovine fibrinogen, another product (III) showed an IC50 (concentration required to double the clotting time relative to a control) of 47 μM.

IT 180152-75-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(low-mol.-weight bicyclic thrombin inhibitors)

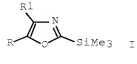
RN 180152-75-4 ZCAPLUS

CN Pyrrolo[1,2-a]pyrazine-6-carboxamide, N-[4-[(aminoiminomethyl)amino]-1-[(5-methyl-2-thiazolyl)carbonyl]butyl]octahydro-4-oxo-2-(1-oxo-3-phenylpropyl)-, [6S-[6α(R*),8aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L31 ANSWER 34 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1987:458912 ZCAPLUS Full-text
DOCUMENT NUMBER: 107:58912
ORIGINAL REFERENCE NO.: 107:9781a,9784a
TITLE: Synthesis and carbodemetalation reactions of 4-methyl- and 5-aryl-2-(trimethylsilyl)oxazoles. Carbon-carbon bond formation at C-2 of the oxazole ring
AUTHOR(S): Dondoni, Alessandro; Fantin, Giancarlo; Fogagnolo, Marco; Medici, Alessandro; Pedrini, Paola
CORPORATE SOURCE: Dip. Chim., Univ. Ferrara, Ferrara, Italy
SOURCE: Dondoni et. al. Journal of Organic Chemistry (1987), 52(15), 3413-20
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:58912
GI



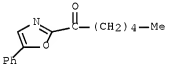
AB The title oxazoles I (R = H, R1 = Me; R = Ph, 4-ClC6H4, 4-MeOC6H4, R1 = H) were prepared by sequential lithiation and silylation of the corresponding substituted oxazoles and isomerization of the resulting α-isocyano silyl enol ethers. I behave as stable 2-oxazolyl anion equivalent toward various carbon electrophiles (aldehydes, acyl chlorides, ketenes, azolium salts) to give 2-substituted oxazoles in good yields.

IT 108665-62-9P 108665-63-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

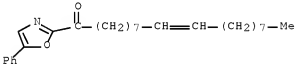
RN 108665-62-9 ZCAPLUS

CN 1-Hexanone, 1-(5-phenyl-2-oxazolyl)- (CA INDEX NAME)



RN 108665-63-0 ZCAPLUS

CN 9-Octadecen-1-one, 1-(5-phenyl-2-oxazolyl)- (CA INDEX NAME)



L31 ANSWER 35 OF 35 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1970:31700 ZCAPLUS Full-text

DOCUMENT NUMBER: 72:31700

ORIGINAL REFERENCE NO.: 72:5801a,5804a

TITLE: Alkylating activity of β-chloroethylamino groups of some 1,3,4-thiadiazole derivatives

AUTHOR(S): Khaletskii, A. M.; Tsurkan, A. A.; Tsurkan, T. S.

CORPORATE SOURCE: Leningrad Chem.-Pharm. Inst., Leningrad, USSR

SOURCE: Farmatsevtichnii Zhurnal (Kiev) (1969), 24(4), 33-7 CODEN: FRZKAP; ISSN: 0367-3057

DOCUMENT TYPE: Journal

LANGUAGE: Ukrainian

GI For diagram(s), see printed CA Issue.

AB I [R1 = Cl(CH2)2NH] (II) were hydrolyzed more quickly than I.HCl. The hydrolysis rate of II increased in the series 4-O2NC6H4 < Ph < 3,4-(MeO)2C6H3 for R2. A reversal sequence was effective for II.HCl. The hydrolysis rate of I [R = p-(Cl-CH2CH2)2NC6H4(CH2)nCO2 nH] (III) increased with increasing n (0-3) and increasing electron-do nor properties of R2. I were determined by titration with 0.1M KOH (phenolphthalein) in 50, aqueous alc. (for II) or hot alc. (for III). The result was checked by the back titration with 0.1M HNO3.

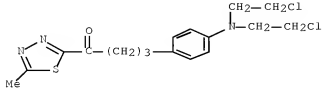
IT 26370-60-5 26370-61-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrolysis of)

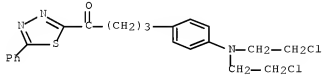
RN 26370-60-5 ZCAPLUS

CN 1-Butanone, 4-[p-[bis(2-chloroethyl)amino]phenyl]-1-(5-methyl-1,3,4-thiadiazol-2-yl)- (8CI) (CA INDEX NAME)

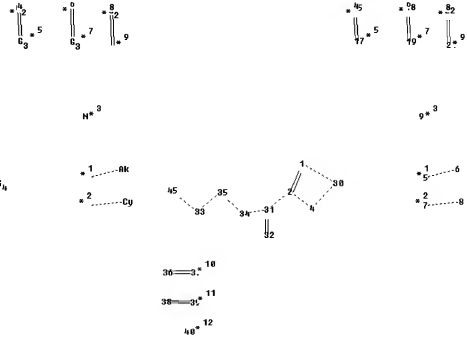


RN 26370-61-6 ZCAPLUS

CN 1-Butanone, 4-[p-[bis(2-chloroethyl)amino]phenyl]-1-(5-phenyl-1,3,4-thiadiazol-2-yl)- (8CI) (CA INDEX NAME)

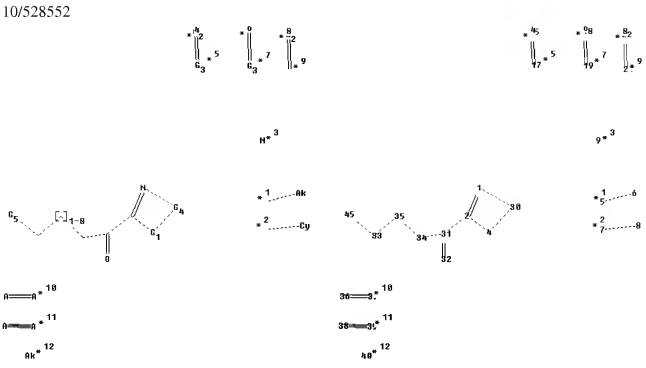


```
=> file registry
FILE 'REGISTRY' ENTERED AT 10:07:19 ON 08 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     7 OCT 2008  HIGHEST RN 1058345-57-5
DICTIONARY FILE UPDATES:    7 OCT 2008  HIGHEST RN 1058345-57-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading L10.str
```



```
chain nodes :
6  8  31  32  33  34  35  40  45
ring nodes :
1  2  4  5  7  9  15  17  18  19  21  22  30
ring/chain nodes :
36  37  38  39
chain bonds :
```

```
2-31  5-6  7-8  31-32  31-34  33-35  33-45  34-35
ring/chain bonds :
36-37  38-39
ring bonds :
1-2  1-30  2-4  4-30  15-17  18-19  21-22
exact/norm bonds :
1-2  1-30  2-4  2-31  4-30  5-6  7-8  15-17  18-19  21-22  31-32  31-34  33-35  33-
45
34-35  36-37
exact bonds :
38-39


G1:O,S

G2:[*1],[*2],[*3]

G3:[*1],[*2]

G4:[*4-*5],[*6-*7],[*8-*9]

G5:[*10],[*11],[*12]

Connectivity :
9:2 E exact RC ring/chain  18:2 E exact RC ring/chain  21:2 E exact RC ring/chain

Match level :
1:Atom  2:Atom  4:Atom  5:Atom  6:CLASS  7:Atom  8:Atom  9:Atom  15:Atom  17:Atom
18:Atom  19:CLASS  21:Atom  22:CLASS  30:Atom  31:CLASS  32:CLASS  33:CLASS
34:CLASS  35:CLASS
36:CLASS  37:CLASS  38:CLASS  39:CLASS  40:CLASS  45:CLASS
Generic attributes :
8:
Saturation             : Unsaturated



Uploading L25.str
```



```
chain nodes :
6  8  31  32  33  34  35  40  45
ring nodes :
1  2  4  5  7  9  15  17  18  19  21  22  30
ring/chain nodes :
36  37  38  39
chain bonds :
2-31  5-6  7-8  31-32  31-34  33-35  33-45  34-35
ring/chain bonds :
36-37  38-39
ring bonds :
1-2  1-30  2-4  4-30  15-17  18-19  21-22
exact/norm bonds :
1-2  1-30  2-4  2-31  4-30  5-6  7-8  15-17  18-19  21-22  31-32  31-34  33-35  33-
45
34-35  36-37
exact bonds :
38-39


G1:O,S

G2:[*1],[*2],[*3]

G3:[*1],[*2]

G4:[*4-*5],[*6-*7],[*8-*9]

G5:[*10],[*11],[*12]

Connectivity :
6:1 E exact RC ring/chain  9:2 E exact RC ring/chain  18:2 E exact RC ring/chain
21:2 E exact RC ring/chain  40:1 E exact RC ring/chain
Match level :
1:Atom  2:Atom  4:Atom  5:Atom  6:CLASS  7:Atom  8:Atom  9:Atom  15:Atom  17:Atom
18:Atom  19:CLASS  21:Atom  22:CLASS  30:Atom  31:CLASS  32:CLASS  33:CLASS
```

```
34:CLASS  35:CLASS
36:CLASS  37:CLASS  38:CLASS  39:CLASS  40:CLASS  45:CLASS
Generic attributes :
8:
Saturation             : Unsaturated



=> file zcaplus
FILE 'ZCAPLUS' ENTERED AT 10:07:21 ON 08 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS is
strictly prohibited.

FILE COVERS 1907 - 8 Oct 2008  VOL 149 ISS 15
FILE LAST UPDATED: 7 Oct 2008  (20081007/ED)

ZCAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L32
L10             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L12         1689 SEA FILE=REGISTRY SSS FUL L10
L25             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L27          373 SEA FILE=REGISTRY SUB=L12 SSS FUL L25
L28           47 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L27
L29          106 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 AND N2COC/ES
L30          267 SEA FILE=REGISTRY ABB=ON  PLU=ON  L27 NOT L29
L31           35 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L30
L32           12 SEA FILE=ZCAPLUS ABB=ON  PLU=ON  L28 NOT L31


=> d ibib abs hitstr L32 1-12
```

L32 ANSWER 1 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:283346 ZCAPLUS Full-text
DOCUMENT NUMBER: 148:299923
TITLE: Methods of correcting bone mineralization defects by using cathepsin B inhibitors and the kits and compositions therefor
INVENTOR(S): Rowe, Peter; Yanagawa, Norimoto
PATENT ASSIGNEE(S): The University of Kansas, USA
SOURCE: Can. Pat. Appl., 80pp.
CODEN: CPXXEB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2558043	A1	20080224	CA 2006-2558043	20060824
AU 2006203680	A1	20080313	AU 2006-203680	20060824
PRIORITY APPLN. INFO.:			CA 2006-2558043	T0 20060824

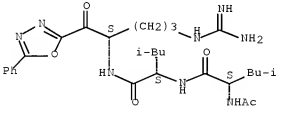
AB The present invention relates to a method of using a therapeutically effective amount of at least one cathepsin B inhibitor for correcting bone mineralization defect. The invention also relates to a combination of the cathepsin B inhibitor with an other agent selected from the group of a second cathepsin B inhibitor, a PHEX polypoeptide, phosphate and calcitriol. Specifically, the invention discloses that the correction of bone miceralization defect includes an increase of d. of pure cortical bone, an increase of mean d. of tatal bone, an increase of cortical thickness , an increase of pure cortical area assigned to be cortical etc.

IT 247209-24-1
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(methods of correcting bone mineralization defects by using cathepsin B inhibitors and kits and compns. therefor)

RN 247209-24-1 ZCAPLUS

CN L-Leucinamide, N-acetyl-L-leucyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (CA INDEX NAME)

Absolute stereochemistry.



L32 ANSWER 2 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:398346 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:124502
TITLE: Keto-1,3,4-oxadiazoles as cathepsin K inhibitors
AUTHOR(S): Palmer, James T.; Hirschbein, Bernard L.; Cheung, Harry; McCarter, John; Janc, James W.; Yu, Z. Walter; Wesolowski, Gregg

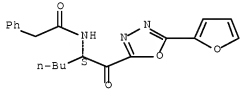
CORPORATE SOURCE: Celera Genomics, Inc., San Francisco, CA, 94080, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(11), 2909-2914
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:124502

AB A series of cathepsin K inhibitors bearing the keto-1,3,4-oxadiazole warhead capable of forming a hemithioketal complex with the target enzyme was prepared By modifying binding moieties at the P1, P2, and prime side positions of the inhibitors, selectivity was achieved over cathepsin B, L, and S, and sub-nanomolar potency was achieved against cathepsin K. This series thus represents a promising chemotype that could be used in diseases implicated by imbalances in cathepsin K activity such as osteoporosis.

IT 896741-34-7 896741-35-8 896741-36-9
896741-37-0 896741-38-1 896741-39-2
896741-40-5
RL: PAC (Pharmacological activity); BIOL (Biological study)
(cathepsin K-inhibiting activity of (keto)oxadiazole derivs.)

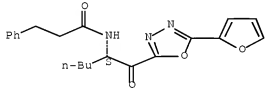
RN 896741-34-7 ZCAPLUS
CN Benzeneacetamide, N-[(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]pentyl]- (CA INDEX NAME)

Absolute stereochemistry.



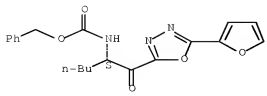
RN 896741-35-8 ZCAPLUS
CN Benzenepropanamide, N-[(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]pentyl]- (CA INDEX NAME)

Absolute stereochemistry.



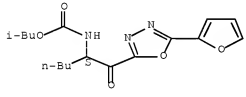
RN 896741-36-9 ZCAPLUS
CN Carbamic acid, [(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]pentyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



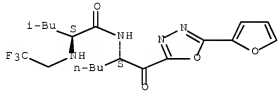
RN 896741-37-0 ZCAPLUS
CN Carbamic acid, [(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]pentyl]-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



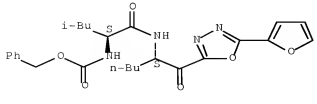
RN 896741-38-1 ZCAPLUS
CN Pentanamide, N-[(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]pentyl]-4-methyl-2-[(2,2,2-trifluoroethyl)amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



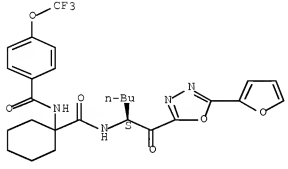
RN 896741-39-2 ZCAPLUS
CN Carbamic acid, [(1S)-1-[[[(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]pentyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



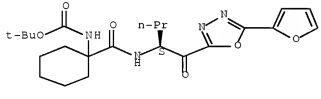
RN 896741-40-5 ZCAPLUS
CN Benzamide, N-[1-[[[(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]pentyl]amino]carbonyl]cyclohexyl]-4-(trifluoromethoxy)- (CA INDEX NAME)

Absolute stereochemistry.



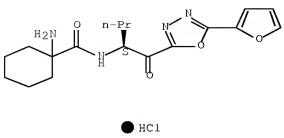
IT 896741-30-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-[(furanyl)oxadiazolyl)carbonyl]butyl](carbamoyl)cyclohexan ecarboxamide derivative and study of its activity as cathepsin K inhibitor)
RN 896741-30-3 ZCAPLUS
CN Carbamic acid, [1-[[[(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]amino]carbonyl]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



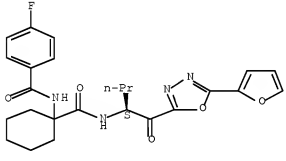
IT 896741-31-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-[(furanyl)oxadiazolyl)carbonyl]butyl](carbamoyl)cyclohexan ecarboxamide derivative and study of its activity as cathepsin K inhibitor)
RN 896741-31-4 ZCAPLUS
CN Cyclohexanecarboxamide, 1-amino-N-[(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]-, hydrochloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.



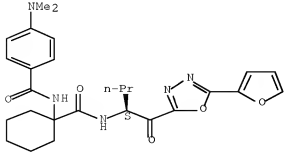
IT 896741-32-5P 896741-33-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of N-[(furanyl)oxadiazolyl)carbonyl]butyl][[(benzoyl)amino]cyclohexanecarboxamide derivs. and study of their activity as cathepsin K inhibitors)
RN 896741-32-5 ZCAPLUS
CN Benzamide, 4-fluoro-N-[1-[[[(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]amino]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 896741-33-6 ZCAPLUS
CN Benzamide, 4-(dimethylamino)-N-[1-[[[(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]amino]carbonyl]cyclohexyl]- (CA INDEX NAME)

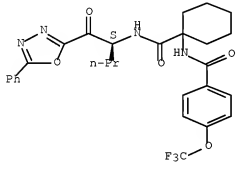
Absolute stereochemistry.



IT 896741-19-8P 896741-20-1P 896741-21-2P
896741-22-3P 896741-23-4P 896741-24-5P
896741-25-6P 896741-26-7P 896741-28-9P
896741-29-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of N-[(oxadiazolyl)carbonyl]butyl][[(trifluoromethoxy)benzoyl]amino]cyclohexanecarboxamide derivs. and study of their activity as cathepsin K inhibitors)

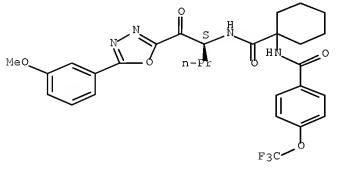
RN 896741-19-8 ZCAPLUS
CN Benzamide, N-[1-[[[(1S)-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]amino]carbonyl]cyclohexyl]-4-(trifluoromethoxy)- (CA INDEX NAME)

Absolute stereochemistry.



RN 896741-20-1 ZCAPLUS
CN Benzamide, N-[1-[[[(1S)-1-[[5-(3-methoxyphenyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]amino]carbonyl]cyclohexyl]-4-(trifluoromethoxy)- (CA INDEX NAME)

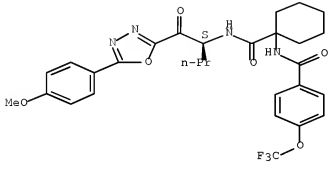
Absolute stereochemistry.



RN 896741-21-2 ZCAPLUS

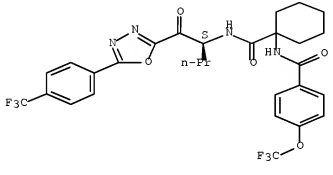
CN Benzamide, N-[1-[[[(1S)-1-[[5-(4-methoxyphenyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]amino]carbonyl]cyclohexyl]-4-(trifluoromethoxy)- (CA INDEX NAME)

Absolute stereochemistry.



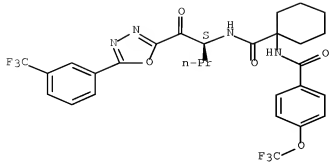
RN 896741-22-3 ZCAPLUS
CN Benzamide, 4-(trifluoromethoxy)-N-[1-[[[(1S)-1-[[5-[4-(trifluoromethyl)phenyl]-1,3,4-oxadiazol-2-yl]carbonyl]butyl]amino]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



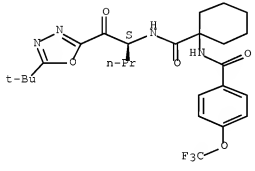
RN 896741-23-4 ZCAPLUS
CN Benzamide, 4-(trifluoromethoxy)-N-[1-[[[(1S)-1-[[5-[3-(trifluoromethyl)phenyl]-1,3,4-oxadiazol-2-yl]carbonyl]butyl]amino]carbonyl]cyclohexyl]- (CA INDEX NAME)

Absolute stereochemistry.



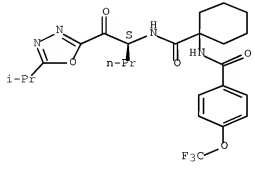
RN 896741-24-5 ZCAPLUS
CN Benzamide, N-[1-[[[(1S)-1-[[5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]amino]carbonyl]cyclohexyl]-4-(trifluoromethoxy)- (CA INDEX NAME)

Absolute stereochemistry.



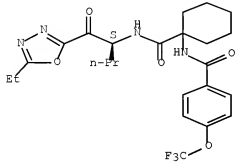
RN 896741-25-6 ZCAPLUS
CN Benzamide, N-[1-[[[(1S)-1-[[5-(1-methylethyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]amino]carbonyl]cyclohexyl]-4-(trifluoromethoxy)- (CA INDEX NAME)

Absolute stereochemistry.



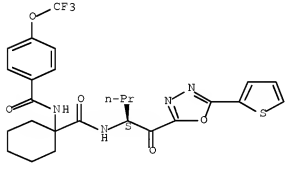
RN 896741-26-7 ZCAPLUS
CN Benzamide, N-[1-[[[(1S)-1-[(5-ethyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]amino]carbonyl]cyclohexyl]-4-(trifluoromethoxy)- (CA INDEX NAME)

Absolute stereochemistry.



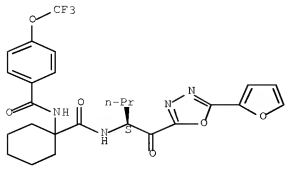
RN 896741-28-9 ZCAPLUS
CN Benzamide, N-[1-[[[(1S)-1-[[5-(2-thienyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]amino]carbonyl]cyclohexyl]-4-(trifluoromethoxy)- (CA INDEX NAME)

Absolute stereochemistry.



RN 896741-29-0 ZCAPLUS
CN Benzamide, N-[1-[[[(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]amino]carbonyl]cyclohexyl]-4-(trifluoromethoxy)- (CA INDEX NAME)

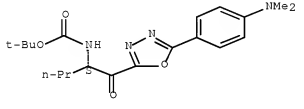
Absolute stereochemistry.



IT 896740-90-2P 896740-91-3P 896740-93-5P
896740-95-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of [(1,3,4-oxadiazolyl)carbonyl]butyl]carbamic acid ester derivs. and study of their activity as cathepsin K inhibitors)

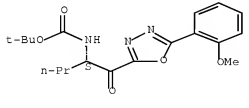
RN 896740-90-2 ZCAPLUS
CN Carbamic acid, [(1S)-1-[[5-[4-(dimethylamino)phenyl]-1,3,4-oxadiazol-2-yl]carbonyl]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



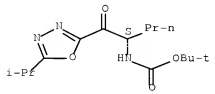
RN 896740-91-3 ZCAPLUS
CN Carbamic acid, [(1S)-1-[[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



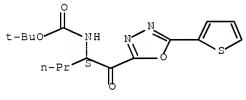
RN 896740-93-5 ZCAPLUS
CN Carbamic acid, [(1S)-1-[[5-(1-methylethyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 896740-95-7 ZCAPLUS
CN Carbamic acid, [(1S)-1-[[5-(2-thienyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:381202 ZCAPLUS Full-text
DOCUMENT NUMBER: 144:412517
TITLE: Oxadiazole ketones as inhibitors of fatty acid amide hydrolase, their preparation, pharmaceutical compositions, and use in therapy
INVENTOR(S): Boger, Dale L.
PATENT ASSIGNEE(S): The Scripps Research Institute, USA
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

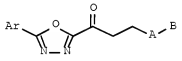
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006044617	A1	20060427	WO 2005-US36963	20051014

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

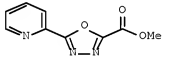
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,

CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

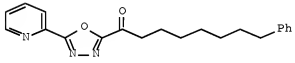
US 20060100212 A1 20060511 US 2005-251317 20051014
US 7351724 B2 20080401
EP 1812427 A1 20070801 EP 2005-808932 20051014
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
US 20080096931 A1 20080424 US 2007-975463 20071019
PRIORITY APPLN. INFO.: US 2004-619172P P 20041015
US 2005-251317 A3 20051014
WO 2005-US36963 W 20051014
OTHER SOURCE(S): CASREACT 144:412517; MARPAT 144:412517
GI



I



II



III

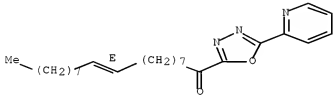
AB The invention relates to oxadiazole ketone compds. of formula I, which are fatty acid amide hydrolase (FAAH) inhibitors. In compds. I, Ar is a 5- or 6-membered aryl or heteroaryl ring having a carbon as its point of attachment; A is a straight-chain C1-7 alkylene having a carbon as its point of attachment to the β-position of the ketone, optionally having 1 or 2 carbon atoms independently replaced by S, O, and/or N; B is C2-10 alkyl, C3-10 cycloalkyl, aryl, C2-10 alkenyl, or C2-10 alkynyl; including pharmaceutically acceptable salts and prodrugs and pharmaceutically active metabolites thereof. The invention also relates to the preparation of I, pharmaceutical compns. comprising a compound I and a pharmaceutically acceptable excipient, optionally containing an analgesic agent, as well as to the use of the compns. for the treatment of a disease, disorder, or condition mediated by FAAH activity, such as anxiety, pain, inflammation, sleep disorders, eating disorders, and movement disorders. Heterocyclization of 2-pyridinecarboxylic hydrazide with Me oxalyl chloride gave oxadiazolecarboxylate II, which underwent substitution with the Grignard reagent prepared from 7-bromoheptylbenzene to give oxadiazole ketone III. The compds. of the invention are inhibitors of FAAH, e.g., compound III expresses IC50 value of 0.6 nM in an assay for FAAH inhibition.

IT 1044713-55-6 1044713-58-7 1044713-59-8

RL: PRPH (Prophetic)
(Oxadiazole ketones as inhibitors of fatty acid amide hydrolase, their preparation, pharmaceutical compositions, and use in therapy)

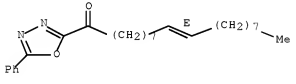
RN 1044713-55-4 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-pyridinyl)-1,3,4-oxadiazol-2-yl]-, (9E)- (CA INDEX NAME)

Double bond geometry as shown.

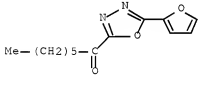


RN 1044713-58-7 ZCAPLUS
CN 9-Octadecen-1-one, 1-(5-phenyl-1,3,4-oxadiazol-2-yl)-, (9E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 1044713-59-8 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]- (CA INDEX NAME)

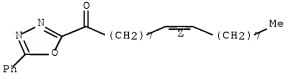


IT 849798-73-8P, (Z)-1-(5-Phenyl-1,3,4-oxadiazol-2-yl)octadec-9-en-1-one 849798-74-9P, (Z)-1-[5-(Pyridin-2-yl)-1,3,4-oxadiazol-2-yl]octadec-9-en-1-one 849798-75-0P, 7-Phenyl-1-(5-phenyl-1,3,4-oxadiazol-2-yl)heptan-1-one 849798-76-1P, 7-Phenyl-1-[5-(pyridin-2-yl)-1,3,4-oxadiazol-2-yl]heptan-1-one 849798-77-2P, 7-Phenyl-1-[5-(pyridin-3-yl)-1,3,4-oxadiazol-2-yl]heptan-1-one 849798-78-3P, 7-Phenyl-1-[5-(pyridin-4-yl)-1,3,4-oxadiazol-2-yl]heptan-1-one 849798-79-4P, 1-[5-(Furan-2-yl)-1,3,4-oxadiazol-2-yl]-7-phenylheptan-1-one 849798-80-7P, 6-Phenyl-1-[5-(pyridin-2-yl)-1,3,4-oxadiazol-2-yl]hexan-1-one 849798-81-8P, 6-Phenyl-1-[5-(pyridin-3-yl)-1,3,4-oxadiazol-2-yl]hexan-1-one

849798-82-9P, 8-Phenyl-1-[5-(pyridin-2-yl)-1,3,4-oxadiazol-2-yl]octan-1-one 849798-83-0P, 9-Phenyl-1-[5-(pyridin-2-yl)-1,3,4-oxadiazol-2-yl]nonan-1-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of oxadiazole ketones as fatty acid amide hydrolase inhibitors)

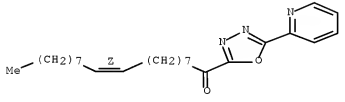
RN 849798-73-8 ZCAPLUS
CN 9-Octadecen-1-one, 1-(5-phenyl-1,3,4-oxadiazol-2-yl)-, (9Z)- (CA INDEX NAME)

Double bond geometry as shown.

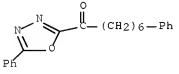


RN 849798-74-9 ZCAPLUS
CN 9-Octadecen-1-one, 1-[5-(2-pyridinyl)-1,3,4-oxadiazol-2-yl]-, (9Z)- (CA INDEX NAME)

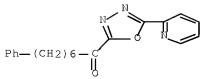
Double bond geometry as shown.



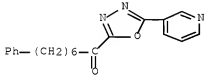
RN 849798-75-0 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-(5-phenyl-1,3,4-oxadiazol-2-yl)- (CA INDEX NAME)



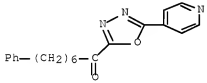
RN 849798-76-1 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(2-pyridinyl)-1,3,4-oxadiazol-2-yl]- (CA INDEX NAME)



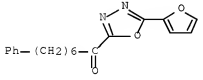
RN 849798-77-2 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(3-pyridinyl)-1,3,4-oxadiazol-2-yl]- (CA INDEX NAME)



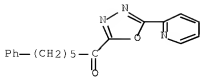
RN 849798-78-3 ZCAPLUS
CN 1-Heptanone, 7-phenyl-1-[5-(4-pyridinyl)-1,3,4-oxadiazol-2-yl]- (CA INDEX NAME)



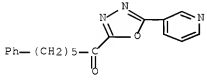
RN 849798-79-4 ZCAPLUS
CN 1-Heptanone, 1-[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]-7-phenyl- (CA INDEX NAME)



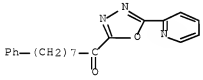
RN 849798-80-7 ZCAPLUS
CN 1-Hexanone, 6-phenyl-1-[5-(2-pyridinyl)-1,3,4-oxadiazol-2-yl]- (CA INDEX NAME)



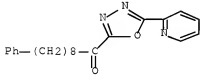
RN 849798-81-8 ZCAPLUS
CN 1-Hexanone, 6-phenyl-1-[5-(3-pyridinyl)-1,3,4-oxadiazol-2-yl]- (CA INDEX NAME)



RN 849798-82-9 ZCAPLUS
CN 1-Octanone, 8-phenyl-1-[5-(2-pyridinyl)-1,3,4-oxadiazol-2-yl]- (CA INDEX NAME)



RN 849798-83-0 ZCAPLUS
CN 1-Nonanone, 9-phenyl-1-[5-(2-pyridinyl)-1,3,4-oxadiazol-2-yl]- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 4 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:376396 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:63134
TITLE: Optimization of subsite binding to the β5 subunit

of the human 20S proteasome using vinyl sulfones and 2-keto-1,3,4-oxadiazoles: Syntheses and cellular properties of potent, selective proteasome inhibitors

AUTHOR(S): Rydzewski, Robert M.; Burrill, Leland; Mendonca, Rohan; Palmer, James T.; Rice, Mark; Tahilramani, Ram; Bass, Kathryn E.; Leung, Ling; Gjerstad, Erik; Janc, James W.; Pan, Lin

CORPORATE SOURCE: Departments of Medicinal Chemistry, Cell Biology, Enzymology, and Distribution Metabolism, and Pharmacokinetics, Celera Genomics, South San Francisco, CA, 94080, USA

SOURCE: Journal of Medicinal Chemistry (2006), 49(10), 2953-2968
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:63134

AB Beginning with the peptide sequence Cbz-Ile-Glu(OtBu)-Ala-Leu found in PSI, a series of vinyl sulfones (VS) were synthesized for evaluation as inhibitors of the chymotrypsin-like activity of the 20S proteasome. Variations at the key P3 position confirmed the importance of a long side chain capped with a hydrophobic group for optimal potency, consistent with a model of binding to the S3 subsite. The tert-Bu glutamic ester initially used at P3 gave plasma unstable, insol. compds. and was replaced with the better isostere, N-β-neopentyl asparagine. The inhibitors were shortened by replacing the N-terminal Cbz-isoleucine with a p-tosyl group without loss of potency. Small L-amino acids were used at P2, where D-substitution was not tolerated. The resulting optimized P4-P3-P2 sequence was grafted onto a novel proteasome inhibitor warhead, 2-keto-1,3,4-oxadiazoles (KOD), to produce reversible, subnanomolar proteasome inhibitors that were 1000-fold selective vs. cathepsin B (CatB), cathepsin S (CatS), and trypsin-like as well as PGPH-like proteasome activity. A number of compds. in both the VS and the KOD series exhibited growth inhibitory effects against the human prostate cancer cell line PC3 at submicromolar concns.

IT 660847-81-4P

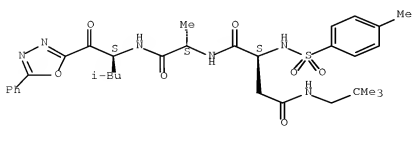
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(solid phase peptide synthesis and proteasome-inhibiting structure-activity relationship of vinyl sulfone and ketoxadiazole peptidomimetics)

RN 660847-81-4 ZCAPLUS

CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

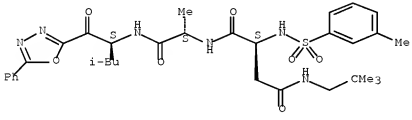
Absolute stereochemistry.



IT 660847-95-0P 660847-99-4P 660848-07-7P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(solid phase peptide synthesis and proteasome-inhibiting structure-activity relationship of vinyl sulfone and ketoxadiazole peptidomimetics)

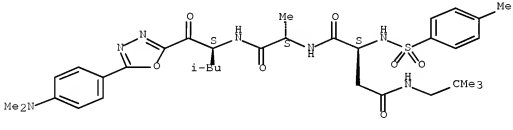
RN 660847-95-0 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(3-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



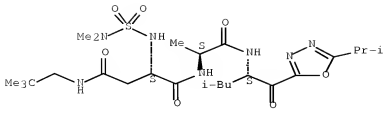
RN 660847-99-4 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-1-[[5-[4-(dimethylamino)phenyl]-1,3,4-oxadiazol-2-yl]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 660848-07-7 ZCAPLUS
CN L-Alaninamide, N2-[(dimethylamino)sulfonyl]-N-(2,2-dimethylpropyl)-L-asparaginyl-N-[(1S)-3-methyl-1-[[5-(1-methylethyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]- (9CI) (CA INDEX NAME)

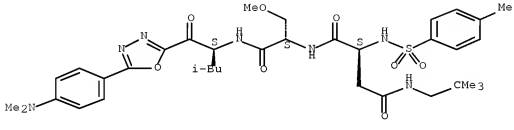
Absolute stereochemistry.



IT 660848-19-1P 660848-23-7P 660848-34-0P
660848-35-1P 890660-61-4P 890660-62-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(solid phase peptide synthesis and proteasome-inhibiting structure-activity relationship of vinyl sulfone and ketoxadiazole peptidomimetics)

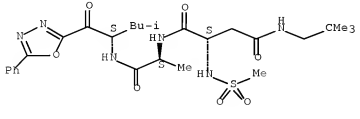
RN 660848-19-1 ZCAPLUS
CN L-Serinamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-1-[[5-[4-(dimethylamino)phenyl]-1,3,4-oxadiazol-2-yl]carbonyl]-3-methylbutyl]-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 660848-23-7 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-(methylsulfonyl)-L-asparaginyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

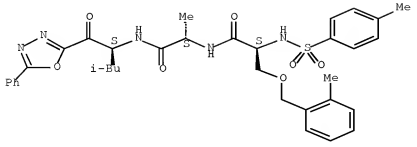
Absolute stereochemistry.



RN 660848-34-0 ZCAPLUS
CN L-Alaninamide, O-[(2-methylphenyl)methyl]-N-[(4-methylphenyl)sulfonyl]-L-seryl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-

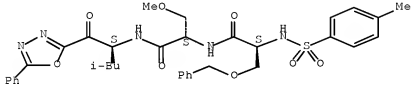
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



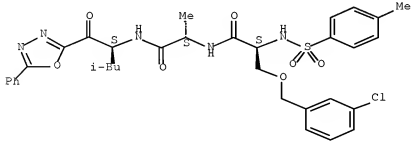
RN 660848-35-1 ZCAPLUS
CN L-Serinamide, N-[(4-methylphenyl)sulfonyl]-O-(phenylmethyl)-L-seryl-O-methyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



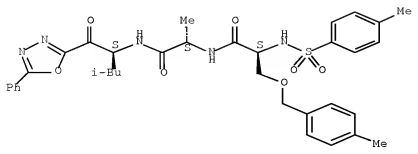
RN 890660-61-4 ZCAPLUS
CN L-Alaninamide, O-[(3-chlorophenyl)methyl]-N-[(4-methylphenyl)sulfonyl]-L-seryl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



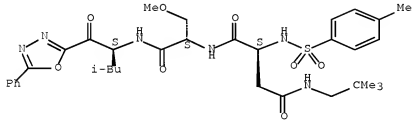
RN 890660-62-5 ZCAPLUS
CN L-Alaninamide, O-[(4-methylphenyl)methyl]-N-[(4-methylphenyl)sulfonyl]-L-seryl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 660847-17-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid phase peptide synthesis and proteasome-inhibiting structure-activity relationship of vinyl sulfone and ketoxadiazole peptidomimetics)
RN 660847-17-6 ZCAPLUS
CN L-Serinamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-O-methyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 5 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:143127 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:193099
TITLE: Heterocyclic compound proteasome inhibitors, pharmaceutical compositions, and therapeutic use
INVENTOR(S): Burrill, Leland C., III; Mendonca, Rohan V.; Palmer, James T.; Rydzewski, Robert M.
PATENT ASSIGNEE(S): Axys Pharmaceuticals, USA
SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004014882	A2	20040219	WO 2003-US24960	20030808
WO 2004014882	A3	20040805		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003255240	A1	20040225	AU 2003-255240	20030808
PRIORITY APPLN. INFO.:			US 2002-402183P	P 20020809
			WO 2003-US24960	W 20030808

OTHER SOURCE(S): MARPAT 140:193099

AB The invention discloses heterocyclic compds. that are proteasome inhibitors, pharmaceutical comprns. comprising such compds., and methods of treating diseases mediated by unregulated proteasome activity. Compound preparation is included.

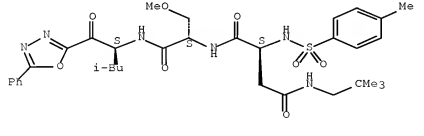
IT 660847-17-6P 660847-77-8P 660847-81-4P
660847-84-7P 660847-87-0P 660847-91-6P
660847-95-0P 660847-99-4P 660848-01-1P
660848-04-4P 660848-07-7P 660848-10-2P
660848-13-5P 660848-15-7P 660848-17-9P
660848-19-1P 660848-21-5P 660848-23-7P
660848-24-8P 660848-26-0P 660848-34-0P
660848-35-1P 660848-38-4P 660848-40-8P
660848-43-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(heterocyclic compound proteasome inhibitors, pharmaceutical comprns., therapeutic use, and use with other agents)

RN 660847-17-6 ZCAPLUS

CN L-Serinamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-O-methyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

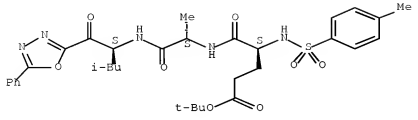
Absolute stereochemistry.



RN 660847-77-8 ZCAPLUS

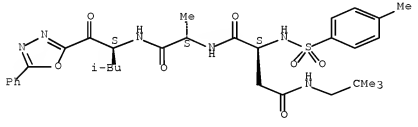
CN L-Alaninamide, N-[(4-methylphenyl)sulfonyl]-L-α-glutamyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



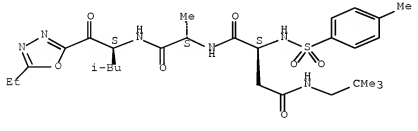
RN 660847-81-4 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



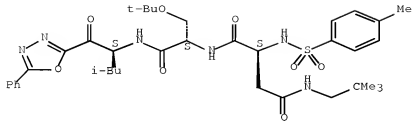
RN 660847-84-7 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-1-[(5-ethyl-1,3,4-oxadiazol-2-yl)carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



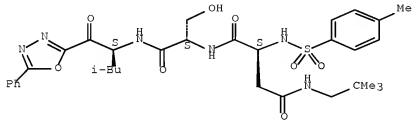
RN 660847-87-0 ZCAPLUS
CN L-Serinamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-O-(1,1-dimethylethyl)-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



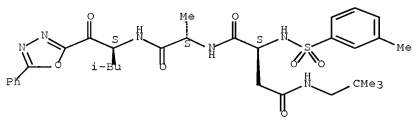
RN 660847-91-6 ZCAPLUS
CN L-Serinamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



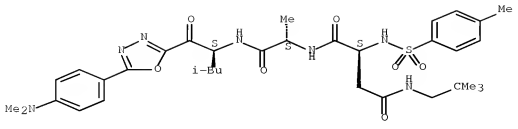
RN 660847-95-0 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(3-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



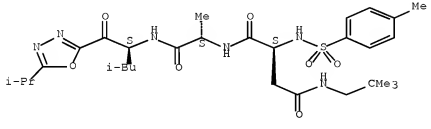
RN 660847-99-4 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-1-[[5-[4-(dimethylamino)phenyl]-1,3,4-oxadiazol-2-yl]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



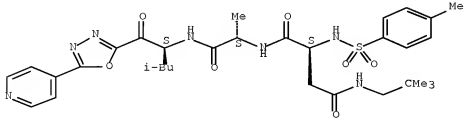
RN 660848-01-1 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-3-methyl-1-[[5-(1-methylethyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



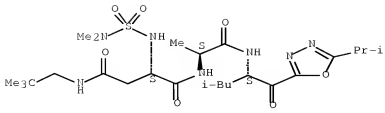
RN 660848-04-4 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-3-methyl-1-[[5-(4-pyridinyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



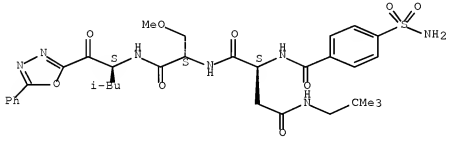
RN 660848-07-7 ZCAPLUS
CN L-Alaninamide, N2-[(dimethylamino)sulfonyl]-N-(2,2-dimethylpropyl)-L-asparaginyl-N-[(1S)-3-methyl-1-[[5-(1-methylethyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



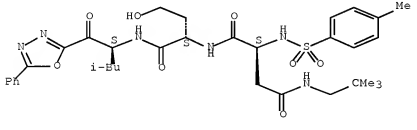
RN 660848-10-2 ZCAPLUS
CN L-Serinamide, N2-[4-(aminosulfonyl)benzoyl]-N-(2,2-dimethylpropyl)-L-asparaginyl-O-methyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



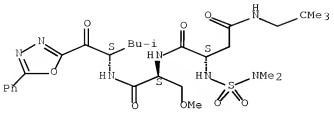
RN 660848-13-5 ZCAPLUS
CN L-Homoserinamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



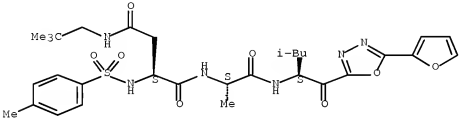
RN 660848-15-7 ZCAPLUS
CN L-Serinamide, N2-[(dimethylamino)sulfonyl]-N-(2,2-dimethylpropyl)-L-asparaginyl-O-methyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



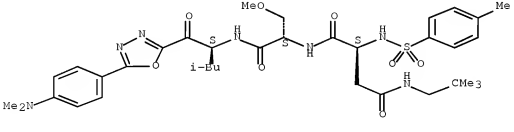
RN 660848-17-9 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-1-[[5-(2-furanyl)-1,3,4-oxadiazol-2-yl]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



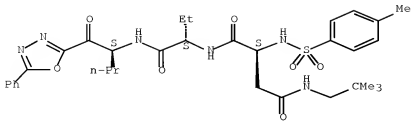
RN 660848-19-1 ZCAPLUS
CN L-Serinamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-1-[[5-[4-(dimethylamino)phenyl]-1,3,4-oxadiazol-2-yl]carbonyl]-3-methylbutyl]-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



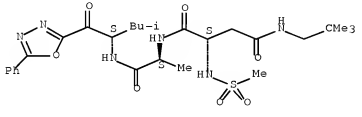
RN 660848-21-5 ZCAPLUS
CN Butanediamide, N4-(2,2-dimethylpropyl)-2-[[(4-methylphenyl)sulfonyl]amino]-N1-[(1S)-1-[[[(1S)-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]amino]carbonyl]propyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



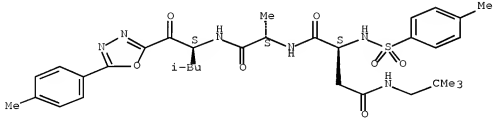
RN 660848-23-7 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-(methylsulfonyl)-L-asparaginyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



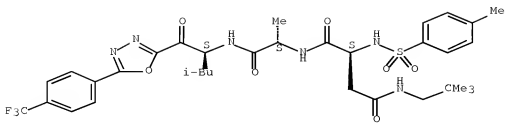
RN 660848-24-8 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-3-methyl-1-[[5-(4-methylphenyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



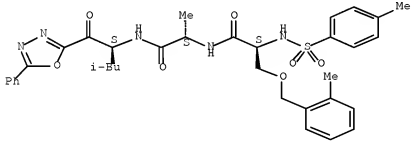
RN 660848-26-0 ZCAPLUS
CN L-Alaninamide, N-(2,2-dimethylpropyl)-N2-[(4-methylphenyl)sulfonyl]-L-asparaginyl-N-[(1S)-3-methyl-1-[[5-[4-(trifluoromethyl)phenyl]-1,3,4-oxadiazol-2-yl]carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



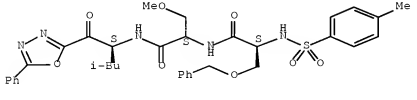
RN 660848-34-0 ZCAPLUS
CN L-Alaninamide, O-[(2-methylphenyl)methyl]-N-[(4-methylphenyl)sulfonyl]-L-seryl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



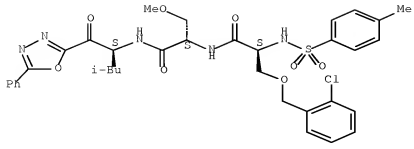
RN 660848-35-1 ZCAPLUS
CN L-Serinamide, N-[(4-methylphenyl)sulfonyl]-O-(phenylmethyl)-L-seryl-O-methyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



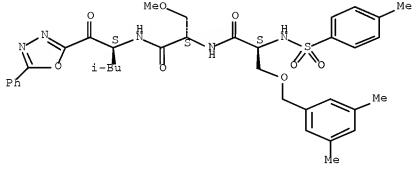
RN 660848-38-4 ZCAPLUS
CN L-Serinamide, O-[(2-chlorophenyl)methyl]-N-[(4-methylphenyl)sulfonyl]-L-seryl-O-methyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



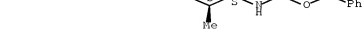
RN 660848-40-8 ZCAPLUS
CN L-Serinamide, O-[(3,5-dimethylphenyl)methyl]-N-[(4-methylphenyl)sulfonyl]-L-seryl-O-methyl-N-[(1S)-3-methyl-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 660848-43-1 ZCAPLUS
CN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-isoleucyl-L-α-glutamyl-N-[(1S)-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L32 ANSWER 6 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:931344 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:5307

TITLE: Preparation of peptides as cysteine protease inhibitors

INVENTOR(S): Graupe, Michael; Lau, Agnes; Link, John O.; Liu, Yang; Mossman, Craig J.; Patterson, John W.; Zipfel, Sheila M.

PATENT ASSIGNEE(S): Axys Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003097617	A1	20031127	WO 2003-US15486	20030514
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2484011	A1	20031127	CA 2003-2484011	20030514
AU 2003234630	A1	20031202	AU 2003-234630	20030514
EP 1503997	A1	20050209	EP 2003-728973	20030514
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006506326	T	20060223	JP 2004-505350	20030514
US 20050288336	A1	20051229	US 2005-514804	20050803
PRIORITY APPLN. INFO.:			US 2002-380311P	P 20020514
			US 2002-422337P	P 20021030
			WO 2003-US15486	W 20030514

OTHER SOURCE(S): MARPAT 140:5307

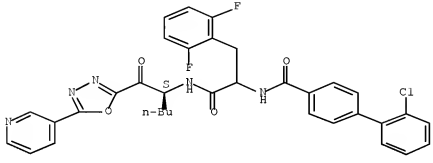
AB The invention is directed to compds. R1CONHCR2R2aCONHCHR3CR4R5R6 [R1 = (hetero)aryl; R2 = H, (cyclo)alkyl, substituted methyl; R2a = H or R2R2aC = cyclohexyl or cycloheptyl; R3 = Et, Pr, Bu; R4 = benzoxazol-2-yl, oxazolo[4,5-b]pyridin-2-yl, 2-pyridin-3-yl[1,3,5]oxadiazol-5-yl, 2-pyridin-4-yl[1,3,4]oxadiazol-5-yl, 2-ethyl[1,3,4]oxadiazol-5-yl, 2-phenyl[1,3,4]oxadiazol-5-yl, pyrazin-2-yl, pyrimidin-2-yl, pyridazin-3-yl, 3-phenyl[1,2,4]oxadiazol-5-yl, or 3-ethyl[1,2,4]oxadiazol- 5-yl; R5 = H, OH, alkoxy; R6 = OH, alkoxy] that are inhibitors of cysteine protease, in particular cathepsins B, K, L, F, and S, and are therefore useful in treating diseases mediated by these proteases. Also disclosed are pharmaceutical compns. comprising these compds. and processes for preparing them. Thus, N-[1(S)-benzoxazol-2-ylcarbonylpropyl]-2-(S)-(2'- chlorobiphen-4-ylcarbonylamino)-3-(2,6-difluorophenyl)propionamide was prepared via amidation of 2-(2'-chlorobiphenyl-4-ylcarbonylamino)-3-(2,6- difluorophenyl)propionic acid with 2(S)-amino-1-benzoxazol-2-ylbutanol (preparation given), followed by Dess-Martin oxidation

IT 627909-73-3P 627909-74-4P 627909-76-6P
627909-79-9P 627909-85-1P 627909-93-7P
627910-08-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptides as cysteine protease inhibitors)

RN 627909-73-3 ZCAPLUS

CN Benzenepropanamide, α-[[(2'-chloro[1,1'-biphenyl]-4-yl)carbonyl]amino]-2,6-difluoro-N-[(1S)-1-[[5-(3-pyridinyl)-1,3,4-oxadiazol-2-yl]carbonyl]pentyl]- (CA INDEX NAME)

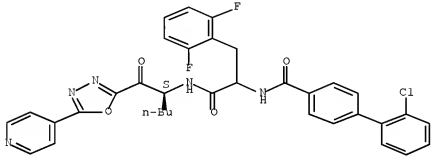
Absolute stereochemistry.



RN 627909-74-4 ZCAPLUS

CN Benzenepropanamide, α-[[(2'-chloro[1,1'-biphenyl]-4-yl)carbonyl]amino]-2,6-difluoro-N-[(1S)-1-[[5-(4-pyridinyl)-1,3,4-oxadiazol-2-yl]carbonyl]pentyl]- (CA INDEX NAME)

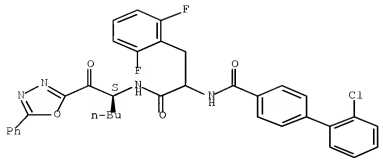
Absolute stereochemistry.



RN 627909-76-6 ZCAPLUS

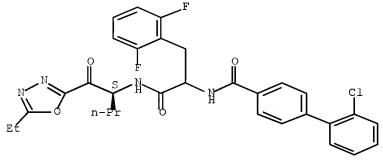
CN Benzenepropanamide, α-[[(2'-chloro[1,1'-biphenyl]-4-yl)carbonyl]amino]-2,6-difluoro-N-[(1S)-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]pentyl]- (CA INDEX NAME)

Absolute stereochemistry.



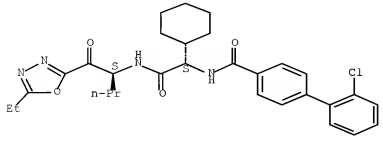
RN 627909-79-9 ZCAPLUS
CN Benzenepropanamide, α-[[(2'-chloro[1,1'-biphenyl]-4-yl)carbonyl]amino]-N-[(1S)-1-[(5-ethyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-2,6-difluoro- (CA INDEX NAME)

Absolute stereochemistry.



RN 627909-89-1 ZCAPLUS
CN [1,1'-Biphenyl]-4-carboxamide, 2'-chloro-N-[(1S)-1-cyclohexyl-2-[[(1S)-1-[(5-ethyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]amino]-2-oxoethyl]- (CA INDEX NAME)

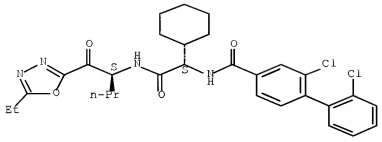
Absolute stereochemistry.



RN 627909-93-7 ZCAPLUS
CN [1,1'-Biphenyl]-4-carboxamide, 2,2'-dichloro-N-[(1S)-1-cyclohexyl-2-[[(1S)-1-[(5-ethyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]amino]-2-oxoethyl]- (CA

INDEX NAME)

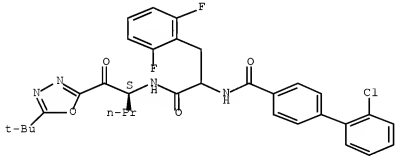
Absolute stereochemistry.



RN 627910-08-1 ZCAPLUS

CN Benzenepropanamide, α-[[(2'-chloro[1,1'-biphenyl]-4-yl)carbonyl]amino]-N-[(1S)-1-[[5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2-yl]carbonyl]butyl]-2,6-difluoro- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 7 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:396872 ZCAPLUS Full-text

DOCUMENT NUMBER: 138:402097

TITLE: Preparation of peptides as cathepsin S inhibitors

INVENTOR(S): Li, Jiayao; Aldous, David J.; Thurairatnam, Sukanthini

PATENT ASSIGNEE(S): Aventis Pharmaceuticals Inc., USA; Axys Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 113 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003042197	A1	20030522	WO 2002-US36396	20021114

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2467391	A1	20030522	CA 2002-2467391		20021114
AU 2002357716	A1	20030526	AU 2002-357716		20021114
US 20030199506	A1	20031023	US 2002-294526		20021114
US 6977256	B2	20051220			
EP 1446392	A1	20040818	EP 2002-792253		20021114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK					
BR 2002014104	A	20040928	BR 2002-14104		20021114
HU 2004001906	A2	20041228	HU 2004-1906		20021114
HU 2004001906	A3	20080728			
CN 1585757	A	20050223	CN 2002-822687		20021114
CN 1324018	C	20070704			
JP 2005514353	T	20050519	JP 2003-544033		20021114
NZ 532167	A	20061130	NZ 2002-532167		20021114
NO 2004001909	A	20040510	NO 2004-1909		20040510
MX 2004PA04450	A	20040811	MX 2004-PA4450		20040511
ZA 2004003602	A	20050831	ZA 2004-3602		20040511
IN 2004CN01053	A	20060203	IN 2004-CN1053		20040513
US 20050267044	A1	20051201	US 2005-166829		20050624
US 7226921	B2	20070605			
HK 1073840	A1	20071221	HK 2005-106311		20050725
US 20070203138	A1	20070830	US 2007-740414		20070426
PRIORITY APPLN. INFO.:			US 2001-332605P	P	20011114
			US 2002-294526	A3	20021114
			WO 2002-US36396	W	20021114
			US 2005-166829	A3	20050624

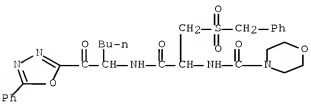
OTHER SOURCE(S): MARPAT 138:402097

AB Peptides R4NHCH(X1-SO2-X2-R3)CONR20CR23R24CO-X3 [X1, X2 are both CH2 or X1 is CH2CH2 and X2 is CH2 or a bond; R3 is (un)substituted CR5:CHR6, CR5(CR63)2, CR7:NR8, or cycloalkyl, where R5 and R6 are H or alkyl or combine to form a (hetero)cycloalkyl, (hetero)aryl, or (hetero)bicycloaryl ring and R7 and R8 combine to form a heterocycloalkyl, heteroaryl, or heterobicycloaryl ring; R4 is an (un)substituted acyl, carboxylate, carbamoyl, sulfonyl, sulfonate, or sulfamoyl moiety; R20 is H, alkyl, (hetero)cycloalkylalkyl or (hetero)arylalkyl; R23 is H or (un)substituted alkyl, alkoxy-, halo-,(hetero)cycloalkyl-, or (hetero)arylalkyl; R24 is H or alkyl; or CR23R24 is (hetero)cycloalkylene; X3 is (un)substituted 1,3,4-oxadiazol-2-yl, 1,2,4-oxadiazol-3(or 5)-yl] or their pharmaceutically-acceptable salts and N-oxides were prepared as novel selective cathepsin S inhibitors. Thus, morpholine-4-carboxylic acid [2-(phenylmethanesulfonyl)-1-[1-(5-phenyl[1,3,4]oxadiazole-2-carbonyl)pentylcarbamoyl]ethyl]amide was prepared by coupling of 2-[(morpholine-4-carbonyl)amino]-3-(phenylmethanesulfonyl)propionic acid with 2-amino-1-(5-phenyl[1,3,4]oxadiazol-2-yl)-1-hexanol TFA salt, followed by oxidation with Dess-Martin periodinane.

IT 530123-06-9P 530123-07-0P 530123-08-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptides as cathepsin S inhibitors)

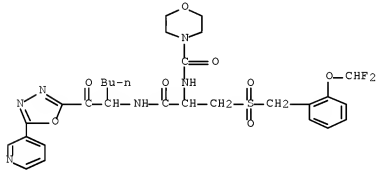
RN 530123-06-9 ZCAPLUS

CN 4-Morpholinecarboxamide, N-[2-oxo-1-[[(phenylmethyl)sulfonyl]methyl]-2-[[1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]pentyl]amino]ethyl]- (CA INDEX NAME)



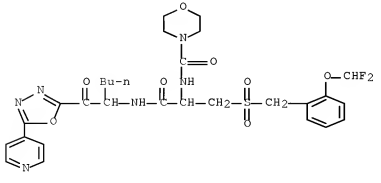
RN 530123-07-0 ZCAPLUS

CN 4-Morpholinecarboxamide, N-[1-[[[[2-(difluoromethoxy)phenyl]methyl]sulfonyl]methyl]-2-oxo-2-[[1-[[5-(3-pyridinyl)-1,3,4-oxadiazol-2-yl]carbonyl]pentyl]amino]ethyl]- (CA INDEX NAME)



RN 530123-08-1 ZCAPLUS

CN 4-Morpholinecarboxamide, N-[1-[[[[2-(difluoromethoxy)phenyl]methyl]sulfonyl]methyl]-2-oxo-2-[[1-[[5-(4-pyridinyl)-1,3,4-oxadiazol-2-yl]carbonyl]pentyl]amino]ethyl]- (CA INDEX NAME)

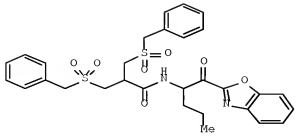


REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 8 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:504904 ZCAPLUS Full-text
DOCUMENT NUMBER: 137:78943
TITLE: Preparation of N-[1-(benzoxazolylcarbonyl)alkyl]- and N-[1-(oxadiazolylcarbonyl)alkyl]alkanamides and related compounds as selective cathepsin S inhibitors
INVENTOR(S): Halley, Frank; Graupe, Michael; Patterson, John; Pickett, Stephen D.; Link, John; Li, Jiayao; Aldous, David; Thurairatnam, Sukanthini; Timm, Andreas; Lai, Justine
PATENT ASSIGNEE(S): Celera, An Applera Corporation Business, USA; Aventis Pharma Inc.
SOURCE: PCT Int. Appl., 724 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002051983	A2	20020704	WO 2001-US50680	20011224
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2433520	A1	20020704	CA 2001-2433520	20011224
AU 2002241728	A1	20020708	AU 2002-241728	20011224
EP 1383748	A2	20040128	EP 2001-988420	20011224
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004523506	T	20040805	JP 2002-553464	20011224
MX 2003PA05601	A	20041202	MX 2003-PA5601	20030620
JP 2008088176	A	20080417	JP 2007-273145	20070920
PRIORITY APPLN. INFO.:			US 2000-257603P P	20001222
			JP 2002-553464 A3	20011224
			WO 2001-US50680 W	20011224

OTHER SOURCE(S): MARPAT 137:78943
GI



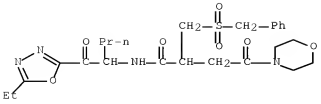
II

AB Title compds. of the formula R3R4CHCONHX1 [I; wherein X1 = CR1R2X2 or X3; X2 = CN, CHO, or (un)substituted (cyclo)alkyl, (hetero)arylalkyl, carbamoylalkyl, aminoalkyl, alkoxyalkyl, sulfamoylalkyl, etc.; X3 = substituted (thi)oxopyrrolidinyl, (thi)oxopiperidinyl, (thi)oxotetrahydro(thio)pyranyl, (thi)oxotetrahydrofuranyl, (thi)oxotetrahydrothiophenyl, etc.; R1 and R2 are both F; or R1 = H or alkyl and R2 = H, alkyl, CN, or (un)substituted amino(alkyl), carbamoyl(alkyl), carboxyamino(alkyl), acyl(alkyl), carboxy(alkyl), sulfamoyl(alkyl), phosphono(alkyl), etc.; or CR1R2 = (un)substituted (hetero)cycloalkyl; R3 and R4 = independently CR16R17X7; R16 and R17 = independently H, alkyl, or F; or R16 = H and R17 = OH; X7 = (un)substituted amino(alkyl), carbamoyl(alkyl), carboxyamino(alkyl), acyl(alkyl), carboxy(alkyl), sulfamoyl(alkyl), etc.; and N-oxides, prodrugs, protected derivs., isomers, pharmaceutically acceptable salts, and solvates thereof] were prepared for treatment of cathepsin S mediated diseases. For example, reaction of 3-benzylsulfanyl-2- benzylsulfanylmethylpropionic acid (preparation given) with 2(S)-amino-1-(benzoxazol-2-yl)-1-pentanol in the presence of HOBt•H2O and EDC in CH2Cl2 afforded the amide. Oxidation of the sulfide groups using Oxone (41%), followed by treatment with Dess-Martin periodinane (74%), gave the title (S)-N-[1-(benzoxazolylmethanoyl)butyl]propanamide (S)-II. I inhibited human cathepsin S protease activity (Ki = 0.1 μM to 0.1 nM) at concns. that were at least 50-fold less than those required to produce an equivalent inhibition of human cathepsin K protease activity. Thus, I are useful for the treatment of diseases mediated by cathepsin S activity, such as autoimmune disorders, disorders involving excessive elastolysis, systemic amyloidosis (no data).

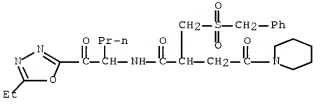
IT 440126-69-2P 440126-71-6P 440126-74-9P
440127-19-5P 440127-27-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(cathepsin S inhibitor; preparation of N-(benzoxazolylcarbonylalkyl)- and N-(oxadiazolylcarbonylalkyl)alkanamides and related compds. as selective cathepsin S inhibitors)

RN 440126-69-2 ZCAPLUS

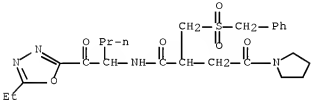
CN 4-Morpholinebutanamide, N-[1-[(5-ethyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-γ-oxo-α-[[(phenylmethyl)sulfonyl]methyl]- (CA INDEX NAME)



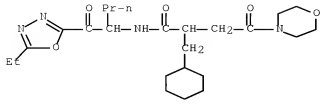
RN 440126-71-6 ZCAPLUS
CN 1-Piperidinebutanamide, N-[1-[(5-ethyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-γ-oxo-α-[[(phenylmethyl)sulfonyl]methyl]- (CA INDEX NAME)



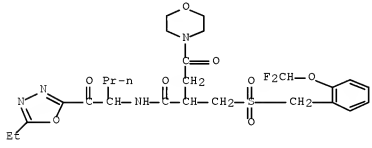
RN 440126-74-9 ZCAPLUS
CN 1-Pyrrolidinebutanamide, N-[1-[(5-ethyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-γ-oxo-α-[[(phenylmethyl)sulfonyl]methyl]- (CA INDEX NAME)



RN 440127-19-5 ZCAPLUS
CN 4-Morpholinebutanamide, α-(cyclohexylmethyl)-N-[1-[(5-ethyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-γ-oxo- (CA INDEX NAME)



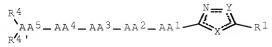
RN 440127-27-5 ZCAPLUS
CN 4-Morpholinebutanamide, α-[[[[2-(difluoromethoxy)phenyl]methyl]sulfo nyl]methyl]-N-[1-[(5-ethyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-γ- oxo- (CA INDEX NAME)



L32 ANSWER 9 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:874195 ZCAPLUS Full-text
DOCUMENT NUMBER: 134:29708
TITLE: Preparation of α-keto heterocycles as serine protease inhibitors
INVENTOR(S): Gyorkos, Albert C.; Spruce, Lyle W.; Leimer, Axel H.; Cheronis, John C.
PATENT ASSIGNEE(S): Cortech, Inc., USA
SOURCE: U.S., 36 pp., Cont.-in-part of U.S. 5,807,829. CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 18
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6159938	A	20001212	US 1997-859242	19970520
US 5618792	A	19970408	US 1994-345820	19941121
US 5807829	A	19980915	US 1996-761190	19961206
US 6037325	A	20000314	US 1998-69823	19980430
PRIORITY APPLN. INFO.:			US 1994-345820	A2 19941121
			US 1996-761190	A2 19961206
			US 1996-698575	A1 19960815

OTHER SOURCE(S): MARPAT 134:29708
GI



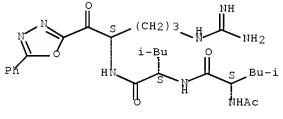
AB Heterocyclyl peptides I [AA1, AA2, AA3, AA4, AA5 are amino acid residues or mimetics or a direct bond; R4, R4' = COR5, CONHR5, SO2R5, CO2R5, CO-(C5-6)aryl-COR5, CH2R5 or R5, where R5 = H, alkyl, alkenyl, (un)substituted alkynyl, cycloalkyl, alkylcycloalkyl, aryl or arylalkyl optionally comprising 1-4 heteroatoms (N, O and S) and optionally substituted, or are absent or R4 and R4' together form a ring comprising 5-7 atoms selected from C, N, S and O; R1 = alkyl or alkenyl optionally substituted with 1-3 halo or hydroxy, alkylamino, cycloalkyl, aryl, etc.; Y, X = O, S, N or substituted N] were prepared for inhibition of serine protease. Thus, N-acetyl-L-leucyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1- [(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]-L-leucinamide (CQ-0002) was prepared and inhibited trypsin with ki = 0.62 nM.

IT 247209-24-1P, CQ 0002
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of α-keto heterocycles as serine protease inhibitors)

RN 247209-24-1 ZCAPLUS

CN L-Leucinamide, N-acetyl-L-leucyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (CA INDEX NAME)

Absolute stereochemistry.

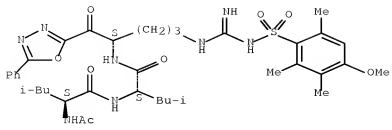


IT 247209-37-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of α-keto heterocycles as serine protease inhibitors)

RN 247209-37-6 ZCAPLUS

CN L-Leucinamide, N-acetyl-L-leucyl-N-[(1S)-4-[[imino[[(4-methoxy-2,3,6-trimethylphenyl)sulfonyl]amino]methyl]amino]-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 10 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:133713 ZCAPLUS Full-text
DOCUMENT NUMBER: 132:180870
TITLE: Preparation of peptidyl α-keto heterocycles as serine protease inhibitors
INVENTOR(S): Gyorkos, Albert C.; Spruce, Lyle W.; Leimer, Axel H.; Cheronis, John C.
PATENT ASSIGNEE(S): Cortech, Inc., USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000009542	A1	20000224	WO 1998-US17449	19980817
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9890315	A	20000306	AU 1998-90315	19980817
EP 1105412	A1	20010613	EP 1998-942211	19980817
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003505008	T	20030212	JP 2000-564992	19980817

PRIORITY APPLN. INFO.: WO 1998-US17449 A 19980817
OTHER SOURCE(S): MARPAT 132:180870
GI

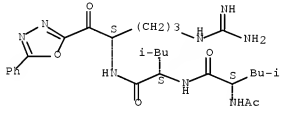
AB Compds. I [Z is a serine protease binding moiety; R1 is an optionally substituted alkyl, alkenyl, cycloalkyl, or aryl group; X, Y = O, S, N or substituted N] were prepared as serine protease inhibitors. Thus, 3-[N-[N-(4-phenylbutanoyl)-L-prolyl]-L-prolyl]-5-(3-phenylpropyl)-1,2,4- oxadiazole (CQ-0006) was prepared by a multistep procedure and showed Ki ≤ 1 nM for inhibition of prolyl oligopeptidase.

IT 247209-24-1P, CQ 0002
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptidyl α-keto heterocycles as serine protease inhibitors)

RN 247209-24-1 ZCAPLUS

CN L-Leucinamide, N-acetyl-L-leucyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (CA INDEX NAME)

Absolute stereochemistry.

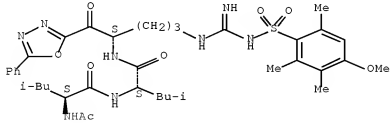


IT 247209-37-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptidyl α-keto heterocycles as serine protease inhibitors)

RN 247209-37-6 ZCAPLUS

CN L-Leucinamide, N-acetyl-L-leucyl-N-[(1S)-4-[[imino[[(4-methoxy-2,3,6-trimethylphenyl)sulfonyl]amino]methyl]amino]-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

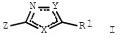
L32 ANSWER 11 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:691089 ZCAPLUS Full-text

DOCUMENT NUMBER: 131:310839
TITLE: Preparation of heterocyclyl peptide derivatives as cysteine protease inhibitors
INVENTOR(S): Spruce, Lyle W.; Gyorkos, Albert C.; Cheronis, John C.; Goodfellow, Val S.; Leimer, Axel H.; Young, John M.; Gerrity, James I.
PATENT ASSIGNEE(S): Cortech Inc., USA
SOURCE: PCT Int. Appl., 90 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9954317	A1	19991028	WO 1999-US8501	19990423
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6004933	A	19991221	US 1998-65258	19980423
CA 2329712	A1	19991028	CA 1999-2329712	19990423
AU 9939651	A	19991108	AU 1999-39651	19990423
AU 750369	B2	20020718		
NZ 507696	A	20031031	NZ 1999-507696	19990423
MX 2000PA10379	A	20010430	MX 2000-PA10379	20001023

PRIORITY APPLN. INFO.:			US 1998-65258	A 19980423
			WO 1999-US8501	W 19990423

OTHER SOURCE(S): MARPAT 131:310839
GI



AB Compds. I (Z is a cysteine protease binding moiety; R1 = alkyl or alkenyl optionally substituted by halo or hydroxy, alkylamino, dialkylamino, alkyldialkylamino, or cycloalkyl, alkylcycloalkyl, alkenylcycloalkyl, aryl, arylalkyl, or arylalkenyl optionally comprising 1-4 heteroatoms selected from N, O and S and optionally substituted by halo, cyano, nitro, amino, alkyl, aryl, etc.; Y, X = O, S, or optionally substituted N) were prepared as cysteine protease inhibitors. Thus, N-[1(S)-[[5-(3- methylbenzyl)-1,3,4-oxadiazol-2-yl]carbonyl]-2-methylpropyl]-L- phenylalaninamide-(3R)-(isobutyl)succinic acid, prepared from 3(S)-[(benzyloxycarbonyl)amino]-2-acetoxy-4-methylpentanenitrile, 3-methylphenylacetic hydrazide, 4-methylvaleric acid, (S)-(-)-4-benzyl-2- oxazolidinone, tert-Bu bromoacetate, tert-butyl-(3R)-3- (isobutyl)succinate, and L-phenylalanine Me ester

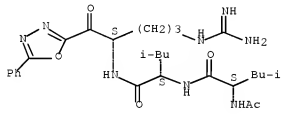
hydrochloride, showed Ki = 85, 3,000, and .apprx.100 nM for inhibition of papain, cathepsin B, and cathepsin L, resp.

IT 247209-24-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclyl peptide derivs. as cysteine protease inhibitors)

RN 247209-24-1 ZCAPLUS

CN L-Leucinamide, N-acetyl-L-leucyl-N-[(1S)-4-[(aminoiminomethyl)amino]-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (CA INDEX NAME)

Absolute stereochemistry.

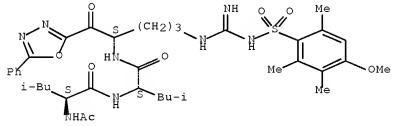


IT 247209-37-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclyl peptide derivs. as cysteine protease inhibitors)

RN 247209-37-6 ZCAPLUS

CN L-Leucinamide, N-acetyl-L-leucyl-N-[(1S)-4-[[imino[[(4-methoxy-2,3,6-trimethylphenyl)sulfonyl]amino]methyl]amino]-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

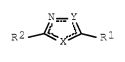
L32 ANSWER 12 OF 12 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:721721 ZCAPLUS Full-text
DOCUMENT NUMBER: 130:4087
TITLE: Preparation of substituted oxadiazole peptide derivatives as cysteine protease inhibitors
INVENTOR(S): Spruce, Lyle W.; Gyorkos, Albert C.; Cheronis, John C.; Goodfellow, Val S.; Leimer, Axel H.; Young, John

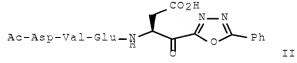
M.; Gerrity, James Ivan
PATENT ASSIGNEE(S): Cortech, Inc., USA
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9849190	A2	19981105	WO 1998-US8259	19980424
WO 9849190	A3	19990218		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9871556	A	19981124	AU 1998-71556	19980424
EP 979242	A2	20000216	EP 1998-918677	19980424
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

PRIORITY APPLN. INFO.: US 1997-44819P P 19970425
US 1998-65258 A 19980423
WO 1998-US8259 W 19980424

OTHER SOURCE(S): MARPAT 130:4087
GI


I


II

AB The present invention relates to cysteine protease inhibitors I [Z = cysteine protease binding moiety, being a carbonyl containing group, preferably an aminocarbonyl containing group, wherein the carbon of the heterocycle is attached directly to the carbonyl group of Z; X, Y = independently O, S or N, where N is optionally substituted with alkyl or alkenyl optionally substituted with 1-3 halo atoms; (C5-C6)aryl, arylalkyl or arylalkenyl optionally comprising 1-3 heteroatoms selected from N, O and S, and optionally substituted with halo, cyano, nitro, haloalkyl, amino, aminoalkyl, dialkylamino, alkyl, alkenyl, alkynyl,alkoxy, haloalkoxy, carboxyl, carboalkoxy, alkylcarboxamide, arylcarboxamide, alkylthio or haloalkylthio; provided that at least one of Y or X = N; R1 = alkyl or alkenyl (un)substituted with 1-3 halo or hydroxy groups; alkylamino, dialkylamino, alkyldialkylamino; cycloalkyl, alkylcycloalkyl, alkenylcycloalkyl, (C5-12)aryl, (C5-12)arylalkyl, (C5-12)arylalkenyl optionally comprising 1-4 heteroatoms N, O and S, and (un)substituted with halo, cyano, NO2, haloalkyl, amino, aminoalkyl, dialkylamino, alkyl, alkenyl, alkynyl, alkoxy, haloalkoxy, carboxyl, carboalkoxy, alkylcarboxamide, (C5-6)aryl, O(C5-6)aryl,

arylcarboxamide, alkylthio or haloalkylthio]. Thus, oxadiazolyl peptide II, prepared in 5 steps from Cbz-Asp(OCMe3)-OH, Ac-Asp(OCMe3)-Val-Gly(OCMe3)-OH, and 2-phenyl-1,3,4-oxadiazole, inhibited caspase 3 with IC50 ≤ 0.1 μM and caspase 6 with IC50 = 6.7 μM. Related oxadiazolyl peptides were prepared and tested for inhibition of caspase 8, caspase 1, granzyme, papain, cathepsin B, cathepsin L, and gingipain R.

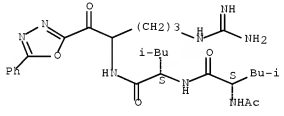
IT 215592-45-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted oxadiazole peptide derivs. as cysteine protease inhibitors)

RN 215592-45-3 ZCAPLUS

CN L-Leucinamide, N-acetyl-L-leucyl-N-[4-[(aminoiminomethyl)amino]-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



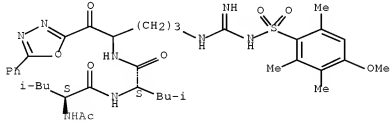
IT 215592-78-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted oxadiazole peptide derivs. as cysteine protease inhibitors)

RN 215592-78-2 ZCAPLUS

CN L-Leucinamide, N-acetyl-L-leucyl-N-[4-[[imino[[(4-methoxy-2,3,6-trimethylphenyl)sulfonyl]amino]methyl]amino]-1-[(5-phenyl-1,3,4-oxadiazol-2-yl)carbonyl]butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



```
=> d his full

     (FILE 'HOME' ENTERED AT 08:54:13 ON 08 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 08:54:22 ON 08 OCT 2008
L1              STRUCTURE UPLOADED
L2           50 SEA SSS SAM L1

     FILE 'ZCAPLUS' ENTERED AT 08:55:42 ON 08 OCT 2008
                E US2005-528552/APPS
L3            1 SEA ABB=ON  PLU=ON  US2005-528552/AP
                D SCA
                SEL RN

     FILE 'REGISTRY' ENTERED AT 08:57:57 ON 08 OCT 2008
L4          136 SEA ABB=ON  PLU=ON  (1006-68-4/BI OR 10200-59-6/BI OR 103-82-2/
                BI OR 109-52-4/BI OR 111-14-8/BI OR 111-64-8/BI OR 112-05-0/BI
                OR 112-13-0/BI OR 112-16-3/BI OR 112-64-1/BI OR 112-67-4/BI OR
                112-76-5/BI OR 112-77-6/BI OR 112-80-1/BI OR 124-07-2/BI OR
                13750-81-7/BI OR 141-75-3/BI OR 142-61-0/BI OR 142-62-1/BI OR
                14436-32-9/BI OR 1484-50-0/BI OR 153301-19-0/BI OR 155601-63-1/
                BI OR 16269-06-0/BI OR 1642-49-5/BI OR 177987-23-4/BI OR
                1821-12-1/BI OR 185444-97-7/BI OR 190131-27-2/BI OR 20662-83-3/
                BI OR 20662-89-9/BI OR 2270-20-4/BI OR 2528-61-2/BI OR
                26547-51-3/BI OR 288862-46-4/BI OR 288862-52-2/BI OR 288862-53-
                3/BI OR 288862-58-8/BI OR 288862-59-9/BI OR 288862-60-2/BI OR
                288862-61-3/BI OR 288862-62-4/BI OR 288862-63-5/BI OR 288862-64
                -6/BI OR 288862-65-7/BI OR 288862-66-8/BI OR 288862-71-5/BI OR
                288862-72-6/BI OR 288862-73-7/BI OR 288862-74-8/BI OR 288862-75
                -9/BI OR 288862-76-0/BI OR 288862-77-1/BI OR 288862-78-2/BI OR
                288862-79-3/BI OR 288862-80-6/BI OR 288862-83-9/BI OR 288862-84
                -0/BI OR 288862-85-1/BI OR 288862-86-2/BI OR 288862-87-3/BI OR
                288862-88-4/BI OR 288862-89-5/BI OR 40228-90-8/BI OR 4091-39-8/
                BI OR 4675-18-7/BI OR 498-60-2/BI OR 498-62-4/BI OR 501-52-0/BI
                 OR 506-24-1/BI OR 544-63-8/BI OR 5581-75-9/BI OR 57-11-4/BI
                OR 638-29-9/BI OR 639819-38-8/BI OR 681135-36-4/BI OR 681135-37
                -5/BI OR 681135-38-6/BI OR 681135-39-7/BI OR 681135-40-0/BI OR
                681135-41-1/BI OR 681135-42-2/BI OR 681135-43-3/BI OR 681135-44
                -4/BI OR 681135-45-5/BI OR 681135-46-6/BI OR 681135-47-7/BI OR
                681135-48-8/BI OR 681135-49-9/BI OR 681135-50-2/BI OR 681135-51
                -3/BI OR 681135-52-4/BI OR 681135-53-5/BI OR 681135-54-6/BI OR
                681135-55-7/BI OR 681135-56-8/BI OR 681135-57-9/BI OR 681135-58
                -0/BI OR 681135-59-1/BI OR 681135-60-4/BI OR 681135-61-5/BI OR
                681135-62-6/BI OR 681135-63-7/BI OR 681135-64-8/BI OR 681135-65
L5          100 SEA ABB=ON  PLU=ON  681135-?/RN
L6           54 SEA ABB=ON  PLU=ON  L4 AND L5

     FILE 'ZCAPLUS' ENTERED AT 09:00:22 ON 08 OCT 2008
L7           18 SEA ABB=ON  PLU=ON  L6
L8              ANALYZE PLU=ON  L7 1- RN HIT :      54 TERMS
                D

     FILE 'REGISTRY' ENTERED AT 09:02:37 ON 08 OCT 2008
L9            1 SEA ABB=ON  PLU=ON  681135-77-3
                D SCA
L10             STRUCTURE UPLOADED
L11          50 SEA SSS SAM L10
                D STAT QUE L11
```

```
L12        1689 SEA SSS FUL L10
                SAVE TEMP CHA552STR10L/A L12
L13          41 SEA ABB=ON  PLU=ON  L12 AND L4

     FILE 'ZCAPLUS' ENTERED AT 09:26:15 ON 08 OCT 2008
L14          18 SEA ABB=ON  PLU=ON  L13

     FILE 'REGISTRY' ENTERED AT 09:28:52 ON 08 OCT 2008
L15             STRUCTURE UPLOADED
L16          44 SEA SUB=L12 SSS SAM L15
L17         753 SEA SUB=L12 SSS FUL L15
                SAVE TEMP CHA552STR15L/A L17

     FILE 'ZCAPLUS' ENTERED AT 09:33:06 ON 08 OCT 2008
L18         143 SEA ABB=ON  PLU=ON  L17
L19             ANALYZE PLU=ON  L18 1- RN HIT :     698 TERMS
                D

     FILE 'REGISTRY' ENTERED AT 09:34:12 ON 08 OCT 2008
L20           1 SEA ABB=ON  PLU=ON  208848-19-5
L21           1 SEA ABB=ON  PLU=ON  208840-24-8
L22           1 SEA ABB=ON  PLU=ON  681135-77-3
L23           1 SEA ABB=ON  PLU=ON  208848-00-4
L24           1 SEA ABB=ON  PLU=ON  208847-80-7
                D SCA L20
                D SCA L21
                D SCA L22
                D SCA L23
L25             STRUCTURE UPLOADED
L26          20 SEA SUB=L12 SSS SAM L25
L27         373 SEA SUB=L12 SSS FUL L25
                SAVE TEMP CHA552STR25L/A L27

     FILE 'ZCAPLUS' ENTERED AT 09:45:08 ON 08 OCT 2008
L28          47 SEA ABB=ON  PLU=ON  L27

     FILE 'REGISTRY' ENTERED AT 09:45:15 ON 08 OCT 2008
L29         106 SEA ABB=ON  PLU=ON  L27 AND N2COC/ES
L30         267 SEA ABB=ON  PLU=ON  L27 NOT L29

     FILE 'ZCAPLUS' ENTERED AT 09:50:18 ON 08 OCT 2008
L31          35 SEA ABB=ON  PLU=ON  L30
L32          12 SEA ABB=ON  PLU=ON  L28 NOT L31

     FILE 'REGISTRY' ENTERED AT 09:57:41 ON 08 OCT 2008
L33          39 SEA ABB=ON  PLU=ON  L27 AND L4

     FILE 'ZCAPLUS' ENTERED AT 10:00:31 ON 08 OCT 2008
L34          10 SEA ABB=ON  PLU=ON  L31 AND P/DT
L35          25 SEA ABB=ON  PLU=ON  L31 NOT L34
L36           6 SEA ABB=ON  PLU=ON  L35 AND PY<2003
L37           5 SEA ABB=ON  PLU=ON  L34 AND PD<20021008
L38           5 SEA ABB=ON  PLU=ON  L34 AND PRD<20021008
L39           5 SEA ABB=ON  PLU=ON  L34 AND AD<20021008
L40          11 SEA ABB=ON  PLU=ON  (L36 OR L37 OR L38 OR L39)
                SEL HIT RN

     FILE 'REGISTRY' ENTERED AT 10:03:22 ON 08 OCT 2008
L41          29 SEA ABB=ON  PLU=ON  (108665-62-9/BI OR 108665-63-0/BI OR
                180152-75-4/BI OR 190523-45-6/BI OR 217457-44-8/BI OR 217457-45
```

-9/BI OR 217457-46-0/BI OR 227962-87-0/BI OR 26370-60-5/BI OR
26370-61-6/BI OR 290817-04-8/BI OR 294882-87-4/BI OR 294882-88-
5/BI OR 294885-02-2/BI OR 294885-03-3/BI OR 294885-04-4/BI OR
321909-54-0/BI OR 321909-55-1/BI OR 321909-59-5/BI OR 321909-60
-8/BI OR 321911-25-5/BI OR 321911-26-6/BI OR 321912-03-2/BI OR
321912-06-5/BI OR 354581-35-4/BI OR 354581-36-5/BI OR 354581-40
-1/BI OR 479420-93-4/BI OR 479421-10-8/BI)

FILE 'REGISTRY' ENTERED AT 10:04:47 ON 08 OCT 2008

FILE 'ZCAPLUS' ENTERED AT 10:04:50 ON 08 OCT 2008
D STAT QUE L31
D IBIB ABS HITSTR L31 1-35

FILE 'REGISTRY' ENTERED AT 10:07:19 ON 08 OCT 2008

FILE 'ZCAPLUS' ENTERED AT 10:07:21 ON 08 OCT 2008
D STAT QUE L32
D IBIB ABS HITSTR L32 1-12

FILE HOME

FILE REGISTRY
Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 6 OCT 2008 HIGHEST RN 1057750-28-3
DICTIONARY FILE UPDATES: 6 OCT 2008 HIGHEST RN 1057750-28-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

FILE ZCAPLUS

Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN. Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS is
strictly prohibited.

FILE COVERS 1907 - 8 Oct 2008 VOL 149 ISS 15
FILE LAST UPDATED: 7 Oct 2008 (20081007/ED)

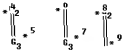
ZCAplus now includes complete International Patent Classification (IPC)

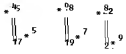
reclassification data for the second quarter of 2008.

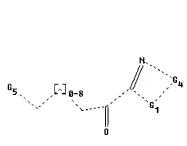
New CAS Information Use Policies, enter HELP USAGETERMS for details.

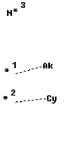
This file contains CAS Registry Numbers for easy and accurate substance identification.

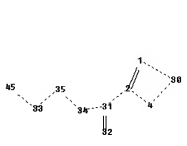
Uploading L10.str

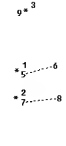












chain nodes :
6 8 31 32 33 34 35 40 45
ring nodes :
1 2 4 5 7 9 15 17 18 19 21 22 30
ring/chain nodes :
36 37 38 39
chain bonds :
2-31 5-6 7-8 31-32 31-34 33-35 33-45 34-35
ring/chain bonds :
36-37 38-39
ring bonds :
1-2 1-30 2-4 4-30 15-17 18-19 21-22
exact/norm bonds :
1-2 1-30 2-4 2-31 4-30 5-6 7-8 15-17 18-19 21-22 31-32 31-34 33-35 33-45
34-35 36-37
exact bonds :
38-39

G1:O,S

G2:[*1],[*2],[*3]

G3:[*1],[*2]

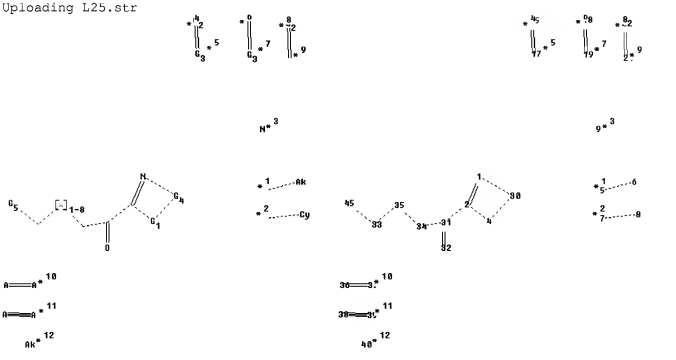
G4:[*4-*5],[*6-*7],[*8-*9]

G5:[*10],[*11],[*12]

Connectivity :
9:2 E exact RC ring/chain 18:2 E exact RC ring/chain 21:2 E exact RC ring/chain

Match level :
1:Atom 2:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom 15:Atom 17:Atom
18:Atom 19:CLASS 21:Atom 22:CLASS 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 35:CLASS
36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 45:CLASS
Generic attributes :
8:
Saturation : Unsaturated

Uploading L25.str



G1:O,S

G2:[*1],[*2],[*3]

G3:[*1],[*2]

G4:[*4-*5],[*6-*7],[*8-*9]

G5:[*10],[*11],[*12]

Connectivity :
6:1 E exact RC ring/chain 9:2 E exact RC ring/chain 18:2 E exact RC ring/chain
21:2 E exact RC ring/chain 40:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom 15:Atom 17:Atom
18:Atom 19:CLASS 21:Atom 22:CLASS 30:Atom 31:CLASS 32:CLASS 33:CLASS
34:CLASS 35:CLASS
36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 45:CLASS
Generic attributes :
8:
Saturation : Unsaturated

=>